Advanced Light Source
Strategic Plan
2015-19

ALS Strategic Plan 2015-19

Executive Summary

We know much about the structure of molecules and solids, yet despite all this knowledge, we still are not able to make the energy storage systems we need, develop efficient artificial photosynthesis, form desired chemical bonds at will, or process information with energy efficiency near the thermodynamic limit. These challenges directly impact problems of major societal importance and will often be addressed using biologically inspired, hierarchical assemblies of cooperatively functioning nanoscale materials. For example, an artificial photosynthesis cell will use a compartmentalized structure to convert solar energy directly to fuel; a catalytic network will arrange nanocatalytic centers in space to perform a multistep chemical synthesis with high efficiency and selectivity; an adaptive material will dynamically redirect the flow of energy to maximize energy storage or control energy conversion efficiency; a neuromorphological processing element might connect multifunctional oxide nanostructures to amplify and use their extreme sensitivity to external stimulus.

Such structures exemplify emergence, in which the function of a composite system is not obviously related to the properties of its atomic and nanoscale components. To understand and ultimately to design structures with emergent properties, we need tools that combine spatial resolution at the nanoscale, where macroscopic properties begin to emerge, with structural, chemical, and magnetic sensitivity, which are directly related to the functional properties we seek. Research with soft x-ray (SXR) beams will be an essential ingredient because we need to use the sharp shallow core levels, the next nearest energy levels to the valence levels we wish to probe, to determine “Where are the electrons?” and “How do they determine chemical bonding, kinetics, magnetism, and many other properties related to useful function?”

Developing predictive power for such emergent properties lies at the core of the 2007 and the 2015 BES Grand Challenges documents and will remain a primary focus of chemical, materials, and biological research for decades to come. How do we rationally assemble multiscale combinations of chemical, material, and biological structures, often with imperfect interfaces and interphases, to achieve a desired function? How do we control non-equilibrium energy, spin, and chemical currents in such assemblies using feedback, regulation, and self-repair to maintain the desired function with high fidelity and efficiency over long periods of time? The vision laid forth in this ALS Strategic Plan is to continue to develop and support cutting edge SXR tools, along with complementary capacity spanning from the infrared through the hard x-ray regime, to probe the structure and function of such hierarchical assemblies.

In its first 22 years of operation the Advanced Light Source (ALS) has lead the world in developing SXR capabilities, including in particular zone plate focusing and advanced spectroscopies in diverse environments. The health of this innovative ALS culture is reflected by current commissioning of a nanoARPES capability to probe the electronic structure at the nanoscale, deployment of new spin-resolved ARPES capability and development of advanced spin detection schemes to probe emerging spintronic materials, current construction of a coherent

SXR scattering beamline to probe nanometer-scale chemical correlations eventually with nanosecond sensitivity, design of new beamlines for advanced energy research and for resonant inelastic scattering, and plans for other new and upgraded capabilities described in this document. It is revealing that demand from the User community for access to the ALS instruments has grown monotonically since commissioning. In particular, demand for Approved Program status, which is a measure of aspirations to form strong partnerships with the ALS and to develop new capabilities like those noted above, has continued to grow even in the past few years, long after the ALS was commissioned.

These ongoing advances in ALS science capabilities have been enabled by a synergistic program of accelerator improvements and upgrades that have allowed the facility to remain at the forefront of x-ray science and technology. This has included, for example, multibunch feedback systems for improved brightness and lower energy spread, superconducting bend magnet sources to provide cost-effective complementary hard x-ray capacity, top-off injection and a sextupole upgrade to increase the source brightness by an additional factor of up to 10, and a pseudo-single-bunch mode to expand ALS capabilities in dynamics experiments. Over the past few years, the ALS Accelerator Physics group has actively participated in the worldwide effort to design ultrahigh brightness storage ring lattices that will produce diffraction limited x-ray beams. A major long-term component of the ALS strategic plan is to upgrade the ALS to a multibend achromat lattice that will provide up to another 1000-fold increase in brightness in the SXR regime. This upgrade, called ALS-U, is absolutely crucial to maintaining ALS world leadership in SXR science for decades to come. It is directly connected to the scientific focus of this strategic plan since material heterogeneity can be encoded into the smooth wave fronts of a diffraction-limited beam. That is, high brightness is directly correlated with our ability to probe the temporal, spatial, and spectral structure of heterogeneous materials and material assemblies.

Though the ALS experimental floor is nearly built out, the facility's innovative culture will continue unabated well into the future by incorporating the latest technologies, continually optimizing and updating existing capabilities, by seeking efficiencies wherever possible, and by repurposing existing beamlines to serve the most relevant science needs. This is particularly important as we start to plan for the new science opportunities that will be afforded by the planned lattice upgrade discussed above. In October 2014, the ALS sponsored a successful workshop focused squarely on these opportunities and a report of the workshop findings has recently been made public. Based on input from that workshop, we are already planning what existing ALS capabilities will need to be upgraded and what new beamlines and instruments will need to be commissioned before the upgrade is complete so we have a suite of instruments ready to take full advantage of the revolutionary new spatial and temporal sensitivities provided by ALS-U. This initial plan for melding ALS priorities with desired ALS-U capabilities is included in the following pages. ALS-U is presently an LBNL Laboratory Initiative and significant laboratory resources are being directed toward this laying groundwork for this potential upgrade.

For example, 2016 LDRD proposals from the ALS and other divisions are heavily focused on planning for ALS-U capabilities.

The ALS works closely with the user community to stay abreast of emerging science areas and to expand the breadth and depth of our experimental capabilities. These interactions are the primary drivers for the demand for General User access and Approved Program status noted above. The ALS is part of the LBNL Energy Sciences Area, the heart of DOE Basic Energy Sciences activity at the laboratory, and regular Area Meetings with partner divisions provide valuable collaborative strategic planning. We have a longstanding partnership with the Chemical Dynamics program in the LBNL Chemical Sciences Division, with the Center for X-ray Optics in the LBNL Materials Science Division, and a growing number of partnerships with the LBNL Molecular Foundry. ALS staff members also collaborate actively through Approved Program agreements with LBNLs Earth Sciences Division, the Joint Center for Artificial Photosynthesis, the Joint Center for Energy Storage Research, and the LBNL Batteries for Advanced Transportation program. Finally, we have an enduring partnership with the LBNL Biosciences Area in protein crystallography, SAXS/WAXS, infrared imaging, and 3D cellular imaging. The ALS also maintains about twenty Approved Program partnerships with users from across the country in areas ranging from high temperature superconductivity to energy and environmental science to high-pressure science. Several EFRCs are included in this group.

The ALS seeks regular advice on its portfolio of instruments and these diverse collaborative research programs through several interrelated activities that feed this Strategic Plan. We engage our Users Executive Committee (UEC) several times per year to discuss how we might help users be more productive at the facility. The UEC also organizes our annual Users Meeting, which includes typically 12-15 topical workshops organized collaboratively by our staff and users. These workshops provide invaluable advice on emerging opportunities and research priorities. User demand is managed with advice from our Proposal Study Panel, which is also actively engaged in evaluating Approved Program Proposals that play such a major role in developing the ALS program. With oversight from our Science Advisory Committee, the ALS organizes typically two reviews per year of entire sub-disciplines to seek focused advice on how to optimize our capabilities to address important research problems. The ALS SAC, composed of national and international experts from many different disciplines, meets twice per year to provide high-level advice on our program.

The excellent ALS staff has established and maintains a productive and highly collaborative environment to accomplish the ALS mission, which is ***to support users in doing outstanding science in a safe environment.*** Motivated by that spirit, this strategic plan outlines a path to a future that is even brighter than our outstanding past.

I. A Synopsis of ALS Strategic Priorities

A. Introduction

Functioning material and biological systems alike often rely on structures that are hierarchical in space and in time. Defects in an oxide gate a few atoms thick govern how efficiently a transistor functions, which in turn determines the power requirements of the gate and how many gates can be placed on a chip. Protein molecules assemble with variable configuration to form the submicron nuclear pore complex to regulate transport through the nuclear membrane, thereby helping to control cell function. But a multiscale structure by itself does not necessarily do anything useful: a complex correlation between different scales is the key ingredient that endows multiscale structures with useful function. Chemical reactions could not occur but for the complex interplay of high energy electronic and low energy vibrational degrees of freedom.

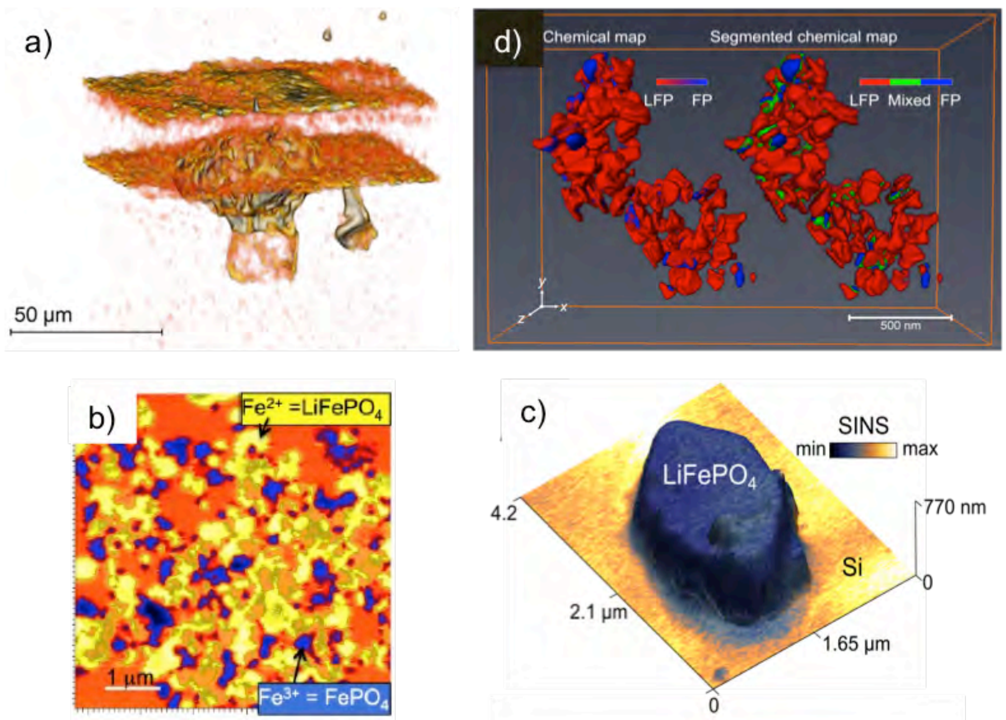

Fig. 1: ALS images spatial scales in lithium ion batteries: (a) Micron scale x-ray tomography of dendrites forming in a model lithium anode (K.J. Harry, et. al., Nature Materials 13, 69-73, (2013)). (b) Oxidation state map of a partially lithiated Li_xFePO_4 cathode measured with a scanning transmission x-ray microscope with ~30 nm resolution (W.C. Chueh et al., *Nano Lett.,* Jan. 30, (2013)). (c) nanoIR imaging combining infrared and atomic force microscopy sensitivities (Hans Bechtel, unpublished) (d) SXR 3D ptychographic reconstruction of grains of a Li_xFePO_4 cathode with 18 nm resolution in all dimensions (David Shapiro, et. al. submitted).

The ALS offers an unmatched suite of multiscale, multimodal imaging tools to probe such hierarchical structures in space (Fig. 1), including ~1 μm resolution hard x-ray and infrared tomography, ~30 nm resolution scanning transmission x-ray microscopy, ~20 nm resolution near field infrared microscopy, and ~10 nm SXR 3D ptychographic imaging with high chemical contrast. ALS staff have achieved 2 nm resolution on 2D test objects using ptychography. An important goal of the ALS COSMIC project is to achieve the spatial and chemical resolution needed to map complex interfaces and interphases in hierarchical structures.

SXR sensitivity extends ALS imaging capabilities to magnetic nanostructures and domains, to orbital structures in complex oxides, to organic photovoltaics, and far beyond. ALS tools have been applied in a pump-probe modality to study multiscale chemical and material dynamics, and the increasing SXR coherent power derived from ongoing ALS accelerator improvements is being leveraged to probe a broad range of spontaneous dynamics as well.

The ALS vision is to continue to support aggressive yet cost effective instrument development activities to address key science areas that crosscut the 2007 and 2015 BES Grand Challenges:

A) *Mapping electronic, ionic, and chemical pathways in catalysis, energy conversion, and energy storage*: utilize the chemical contrast and spatial resolution of SXR spectromicroscopy to probe structure-function relationships in operating, hierarchical catalytic processes and energy devices

B) *Enabling development of new functional materials for ultralow power electronics:* utilize the spatial sensitivity, spectral contrast, and temporal resolution of ring-based SXR beams in support of emerging classical, quantum, magnetic, spintronic, and neuromorphic information processing technologies

C) *Illuminating the crossover between dynamics and kinetics at the nanoscale*: develop tools and protocols to understand how bond breaking and spin flips connect, for example, to activated chemical kinetics and domain wall motion to develop selective and efficient materials synthesis, self-assembly, and function

D) *Understanding complex biological and environmental interactions across large temporal and spatial scales*: harness the power of existing and emerging ALS imaging and spectroscopic tools to understand natural processes at their most relevant length and time scales.

E) *Developing experimental protocols that use high SXR coherence to understand new material phases and phenomena*: learn how to leverage phase coherence provided by modern storage ring sources to vastly improve the sensitivity, spectral resolution, and spatial and temporal dynamic range of SXR techniques

Since 1993, the ALS has emerged as the world leader in SXR science while also offering complementary infrared and hard x-ray capabilities. The facility owes its success to its deep connection to current research trends, driven by strong partnership with an outstanding user community, with other LBNL divisions, and with University of California Berkeley faculty. These partnerships drive continued invention and innovation in instrumentation, a successful program of accelerator upgrades, a strong commitment to user support, and constant attention to all aspects of safety. The facility supports the research of over 2400 users per year whose results appeared in >800 refereed journal publications in 2014, with over 150 articles in high-impact journals. The ALS has 40 beamlines and operates more than 5,000 hours each year.

Though the ALS is nearly built out, its innovative culture will continue unabated well into the future by continually upgrading the accelerator to enable more incisive tools, by optimizing existing tools, by seeking efficiencies wherever possible, and by repurposing existing beamlines to serve the evolving science needs of our diverse user community. Sec. II of this Strategic Plan examines how the ALS will marshal its resources to develop tools that continue to enable new and important science. Sec. III discusses ongoing and proposed accelerator upgrades that serve ever more powerful tools. The research themes bulleted above, as well as the strategic plan for beamlines, end stations, and accelerator upgrades discussed below, have been developed and prioritized through extensive engagement with the ALS user community through workshops, cross-cutting reviews, and advisory committees, as explained in Sec. IV.D.

In the remainder of this introductory section, we tabulate and briefly describe of ALS strategic priorities for 2015-19 in the areas of beamlines and end stations (Sec. I.B), accelerator upgrades and improvements (Sec I.C), and other ancillary capabilities (Sec. I.D). ALS-U is not yet a project, but encouraging words from BES staff has motivated us to discuss long range plans for ALS-U in Sec. I.E of this ALS strategic plan. In Sec. II, we describe in greater detail ALS beamline and end station projects and priorities listed in Sec. I.A in greater detail. Sec. III elaborates our plans for accelerator improvements and upgrades, including a brief description of ALS-U. In Sec. IV we describe ancillary activities that draw on ALS resources to increase our productivity and safety.

B. Instruments to Address High Impact DOE Research Problems

Table 1 on the next two pages summarizes ALS strategic beamline and end station projects having a total cost typically in excess of \$0.5M. The table delineates projects that are being commissioned, are under construction, are being designed, or are our highest priority unfunded projects planned over a longer time scale. Only projects in the last group lack estimated cost and schedule (not shown here). The table also indicates the diversity of partners that are helping to develop the ALS program by contributing financially to these projects (note that a list of acronyms can be found in Appendix 1).

The sixth column of Table 1 links the various beamline and end station projects to the five key science areas in the above bullets and discussed in greater detail in the subsections II.A – II.E. Each subsection briefly explains the importance of a particular research area, indicates how SXR science and technology will play a major role in addressing key underlying issues, examines existing ALS capabilities relevant to the area, and discusses how near- and long-term beamline and end station strategic plans provide crucial future capacity and capabilities.

While the ALS continues to innovate new and to upgrade existing capabilities, the facility carefully balances its suite of instruments with the staff it is able to support so as to maintain efficient and sustainable operations. The ALS maintains a spreadsheet of beamline metrics that provides a snapshot of beamline staffing, user demand, usage, operational complexity, and overall productivity. This is used to help maintain an appropriate level of support on different beamlines. We increasingly train our staff across different beamlines to enhance operational efficiency. Most of the projects listed in Table 1 are net-staffing-neutral.

Table 1. ALS Major Beamline and End Station Projects, 2015-19

Beamline	Project Title	Project Scope	Commission year	Partners & Funding	Section II thrusts	Notes
7.0.2	MAESTRO	new undulator, beamline, end stations	underway	SISGR ALS ops	B	Half-length undulator and high resolution SXR beamline with ARPES, nanoARPES, and PEEM end stations; extensive film growth and analysis capabilities
4.0.2	High field magnetic spectroscopy	new end station	underway	ARRA	B	High field (5T) magnetic spectroscopy end station, variable field orientation; low temperature sample stage
10.0.1.2	spinARPES	new refocus optics, new end station	2015	ALS ops	B	Spin-resolved ARPES end station with enhanced exchange-scattering detectors to enables energy high-resolution; film growth capability; new refocus optics on repurposed beamline
2.4	Infrared microscopy & tomography	new beamline, front end, optics	2015	SUFD ALS ops	D	Infrared beamline for spectromicroscopy, primarily of environmental and biological samples; focal plane array detector will allow IR tomography
9.3.1	HAXPES	upgrade optics, new mono	2016	JCAP, JCESR, BATT, ALS ops	A	Upgrade tender energy beamline for high energy photoemission; ambient pressure XPS at the solid/solid and solid/liquid interface; new crystal monochromator; smaller focal spot for higher pressure operation
7.0.1.1 7.0.1.2	COSMIC	new undulator, beamlines, end stations	2016	DMSE, DOE midscale ALS ops	A, B, C, E	New half-length undulator and moderate-resolution SXR beamlines for coherent scattering and imaging; mesoscale 3D chemical imaging; XPCS studies of spontaneous fluctuations in complex magnetic systems
12.2.1	Chemical & materials crystallography	move program to superbend, new robot	2016	LBNL/MF ALS Ops	A	100x higher flux at high energy than present home at 11.3.1; diverse sample environments; robot for efficient material screening; partnering with MF
9.0.1	Chemical dynamics	install used SXR mono from SRC	2016	CSBG, LBNL/CSD	C	Configure and install modern monochromator from Wisconsin/SRC; expands chemical dynamics program into SXR regime; allows flexible studies of dynamics and kinetics
7.3.1	SXR spectroscopy	upgrade mono, restart BL	2016	JCAP, ALS ops	A	Rebuild bend magnet beamline; update grating, install new slits; increases capacity for SXR spectroscopy; complements existing undulator-based capacity
5.3.1	T-REXS	repurpose beamline, end station	2016	LDRD, NIH LBNL/PBD	A, D	Repurpose existing R&D beamline for tender energy scattering of material and biological samples; 2015 and 2016 LDRD project, new high frame rate detector supported by NIH
2.0	GEMINI	new undulator, beamline, end station	2017	HHMI, LBNL, LBNL/PBD/NIH	D	High-brightness cryogenic undulator and crystal monochromator; microfocus optics into two diffractometers operating in parallel; macromolecular crystallography with small crystals and large unit cells; advanced detectors; robotic sample handling
6.0.1	QERLIN/RIXS	repurpose undulator, new beamline and ES	2018	Moore Foundation, ALS ops	B, C, E	Soft x-ray RIXS beamline and end station to probe coupled excitations in complex electronic materials; double dispersion design to provide ~100x higher throughput that existing designs
6.0.2	AMBER/SXR spectroscopy	Repurpose undulator, new beamline and ES	2018	PNNL, JCAP BATT, JCESR, ALS ops	A, B	Energy materials beamline; initially soft x-ray spectroscopy; STXM, APXPS to be developed; diverse and flexible sample environments

4.0.2	Magnetic STXM	new end station	2018	NSF-MRI/UCB?	B	STXM/ptychography end station for magnetic materials, complex oxides; fields to 2-3 T, variable temperature precision sample stage
4.0.2	Magnetic spectroscopy	upgrade undulator, beamline	2018	ALS ops?	B	Upgrade 16 year old beamline, 10x more flux and much higher brightness at ALS; ALS-U ready; modern monochromator; optics upgrade; optimized undulator period
	SAXS	move 7.3.3 SAXS/WAXS to SB/wiggler	2018	ALS ops?	A	Move existing SAXS beamline to a SB; 100x increase in flux and capacity; increase time resolution and install crystal monochromator for lower energy band width; diverse sample environments.
	Nano-spinARPES	planning	202x	Conceptual design with LDRD	B	With LDRD support, ALS is planning to combine growing expertise in nanoARPES with advanced spin detectors to probe the spin structure in nano-devices and nano-structured materials. Benefits heavily from ALS-U
9.0	Chicane sector, update optics	planning	202x		C	Doubles capacity and serves VUV and soft x-ray chemical dynamics/kinetics beamlines; a key part of ALS-U planning; will need to wait to on-axis injector so a new class of high brightness undulator can be deployed
10.0	Chicane sector, update beamlines	planning	202x		B	Increase ARPES capacity; likely home for nano-spinARPES above; a key part of ALS-U planning; will need to wait to on-axis injector so a new class of high brightness undulator can be deployed
8.0	Chicane sector, update beamlines	planning	202x		A	Two high performance undulators for soft and intermediate energy spectroscopy and microscopy; probably done in sync with ALS-U

Commission   Construct   Design & Procure   Future planning/not funded

*** List of acronyms is provided in Appendix 1**

C. Accelerator Upgrades to Enable Improved ALS Tools

Cutting-edge instruments provide only part of what is required for continuous ALS renewal and thus do not capture the totality of the ALS innovative spirit. Current strategic priorities for the existing ALS accelerator for 2015-19 and initial R&D priorities for the proposed ALS upgrade (ALS-U) are summarized in Table 2 and are further elaborated in Sec. III.

The ALS is emerging from a phase of renewal that modernized most major existing accelerator systems: power supplies, control systems, rf system, and a host of smaller components. Conversion to top-off operation and addition of 48 sextapoles to the lattice has increased source brightness by an order of magnitude in the past 7 years. As indicated in Table 2, replacement and upgrade of other accelerator and injector subsystems continues apace.

Finally, a crucial long-term focus of our strategic plan, which will ensure continued ALS world-leadership in soft x-ray science and technology for decades to come, is to replace the ALS accelerator with a multibend achromat (MBA) lattice that will provide ultrabright, diffraction-limited soft x-ray beams up to ~2keV. This planned upgrade is in perfect sync with the science areas discussed in Sec. II since there is a direct relationship between source transverse coherent power and our ability to probe multiscale heterogeneous systems.

Table 2: ALS Accelerator R&D and Construction Projects, 2015-19

Project	Commission year	Funding source	Notes
ALS RF Upgrade	2014-15	SUFD ALS ops	Update aging RF system; eliminate potential major single-point failures (nearly complete)
ALS Controls Upgrade	2014-15	SUFD ALS Ops	Update aging storage ring control system (nearly complete)
Booster ring rf modulators	2016	ALS Ops	
ALS-U R&D	2014-202x	SUFD LDRD	R&D on non-evaporable getter coatings on small diameter vacuum chambers, fast kicker magnets for on axis injection, optics to focus diffraction-limited SXR beams, on-axis injector, MBA lattice, high performance undulators
AC power conditioning	2018	DOE LBNL	2 MW power conditioning system to address external power glitches and to improve ALS reliability
HVAC upgrade	2019	DOE LBNL	Stabilizes ALS environment for improved beam stability

D. Ancillary Capabilities to Support a Strong User Science Program

Table 3 summarizes several enabling ALS programs and technologies that support our strategic research priorities and engage the user community in strong partnerships. These include establishing efficient procedures to optimize facility usage, maintaining a strong safety culture, focusing on ALS staff professional development, engaging users in the strategic planning process, testing and regularly upgrading beamlines and optics, developing nanodiffractive optics that support advances many ALS capabilities, developing and deploying state of the art x-ray detectors, building the infrastructure needed to manage and to analyze the huge volume of data produced at the ALS. These are managed strategically and balanced against other instrument and accelerator needs, and are described in more detail in Sec. IV.

Table 3. Ancillary Activities Supported by ALS, 2015-19

Project	Commission	Funding Source	Notes
User Portal	2014-5	ALS Ops	Complete modern portal to manage user access and to ensure their safe operation at the ALS
LUXOR	ongoing	ALS Ops	Ongoing optics upgrade for older ALS beamlines; 1-2 beamlines per year
Diffractive Optics	ongoing	ALS Ops	Support work with the CXRO and Molecular Foundry for nano-diffractive optics, used on 6 ALS beamlines now, growing to ~12 on ALS-U
Optical Metrology Lab	2014-5	SUFD, ALS Ops	Purchase new instruments and support ALS Optical Metrology Lab, to ensure efficient use of high brightness x-ray beams
Scientific Data Management	ongoing	ALS Ops BES/ASCR	Work with LBNL computing divisions to maintain and expand our ability to transmit, store, manage, and analyze large data streams
Advanced Detectors	ongoing	ALS Ops	Continue development of detectors with high frame rate, high spatial resolution, or other specific characteristics
Fellowship programs	ongoing	ALS Ops	Ongoing support of ALS Post baccalaureate, Doctoral, and Postdoctoral Fellowship Programs for professional and staff development

E. Preliminary Strategic Planning for the ALS – ALS-U transition

The ALS Upgrade discussed briefly above and in more detail in Sec. III is at least 6-7 years from commissioning, but advanced planning has been underway for some time. ALS-U is an LBNL Labwide Initiative, and the laboratory is channeling resources to help plan and reduce risk for this proposed project. ALS staff have been actively engaged in activities focused on ALS-U, some of which were included in Table 2 above. Preliminary conceptual design and cost estimate will be available in the next 6-12 months. Initial planning for the roughly one-year shutdown to remove the ALS accelerator and to install the MBA ALS-U undulator is underway.

A key feature of the planning process for ALS-U is to ensure the new lattice can be commissioned with a full complement of recently upgraded or new beamlines that are ready to take advantage of the huge increase in source brightness. Key features of this emerging proposed plan for beamline upgrades include:

- The on-axis injection scheme for ALS-U will enable an entirely new class of narrow gap and shorter period undulators that are a key component needed to achieve the highest possible brightness. It will be possible to start upgrading undulators when the new injector is commissioned, which is presently planned to occur after the first 2-3 years of the proposed ALS-U project. The new class of undulators is expected to be less expensive than existing ALS undulators, and we hope to start replacing undulators a few years before ALS-U is commissioned – to be ready for the ALS-U science program.
- Even though they have been continually upgraded, undulator beamlines that are currently more than 10-15 years old will be approaching the end their useful lives when ALS-U is commissioned. These will therefore need to be replaced or seriously upgraded for either ALS or ALS-U operation. These are listed as open-ended strategic priorities in Table 1. We are working on ways to help fund these upgrades.
- ALS undulator beamlines constructed in the last 5-10 years are based on modern optical designs and have been maintained and upgraded regularly. They are mostly ALS-U ready, except a new generation of coherence-preserving optics will be needed to handle diffraction-limited SXR photon beams from ALS-U. Establishing the design parameters of such optics, especially how to handle the high power density, is presently being initiated with LDRD funding (Table 2).
- Conceptualizing, designing and building new state of the art end stations is a constant process at the ALS; note for example that many entries in Table 1 describe end station projects. These capabilities are being planned with ALS-U very much in mind.

Accomplishing the accelerator, undulator, beamline, end station, and optics upgrades listed above will preserve or expand all existing ALS capabilities in a very cost effective fashion.

II. ALS Blue: Tools to Probe Functional Materials and Devices

A. Mapping Chemical and Energy Pathways

Devices currently in use or being developed for selective and efficient heterogeneous catalysis, photocatalysis, energy conversion, and energy storage rely heavily on diverse multiscale phenomena, ranging from interfacial electron transfer and ion transport occurring on nanometer - picosecond scales to macroscale batteries that charge in hours and catalytic reactors with turnover rates of ~1/sec. Soft and hard x-rays can probe dense environments with atomic and chemical contrast spanning a large spatiotemporal range, thereby providing unique fundamental information about functioning mesoscale devices. For example, ALS staff have collaborated with user groups develop and apply tools to map key chemical structures in batteries (Fig. 1) in real time during charging cycles. Such 'nanokinetic' measurements are essential to optimize such complex multiscale (electro)chemical devices.

The number of current ALS beamlines used for energy science and catalysis research is extensive. Many of these are among our most heavily over-subscribed beamlines and Table 1 indicates that our strategic priorities increase both our capability and our capacity to help users study energy conversion, energy storage, and catalytic materials. These are explained more fully below:

1. Cutting edge spectromicroscopy: COSMIC

Since 1995, the ALS has led the world in developing soft x-ray scanning transmission x-ray microscopes (STXMs), and STXMs on ALS beamlines 5.3.2.1/2 and 11.0.2 are highly productive. Commissioning of the COherent Scattering and MICrscopy beamline (COSMIC) in early 2016 will maintain this world leadership. One branch of COSMIC will do ptychographic diffractive imaging with state-of-the-art scanning systems, high-data-rate CCD detectors matched to a high bandwidth data system, and diverse *in situ* sample environments. The precursor of COSMIC provided the image in Fig. 1(d). COSMIC will provide few-nanometer resolution images, ultimately combining 3D tomographic reconstruction with full chemical contrast. Among many other areas, this will revolutionize our ability to probe 'interphase' regions like the solid-electrolyte interphase that governs the operation of batteries, fuel cells, and other electrochemical systems as well as photocatalytic reactors used for artificial photosynthesis. A new approved program will help bring TEM sample environments to this new facility to support users studying diverse chemical systems.

2. Soft and Intermediate Energy X-ray Spectroscopy: AMBER, update 7.3.1, 9.3.1

In addition to the advanced imaging capabilities exemplified by COSMIC, ALS development of *in operando* sample-handling systems, high throughput x-ray emission spectrographs, and ambient pressure x-ray photoelectron spectroscopy (APXPS) has attracted many users wanting to tackle key basic science issues in catalysis and energy sciences. Soft x-ray absorption (XAS) and emission (SXE) spectroscopies on beamline 8.0.1 provide a direct probe of a material's

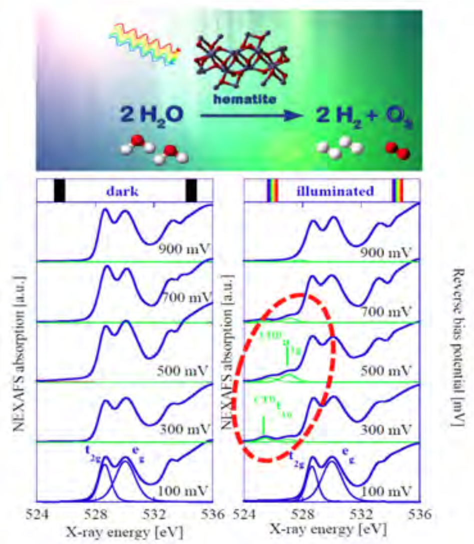

Fig. 2. Electron-hole formation at the hematite/ water interface upon absorption of light. A. Braun et al., *J. Phys. Chem C* **116**, 16870 (2012).

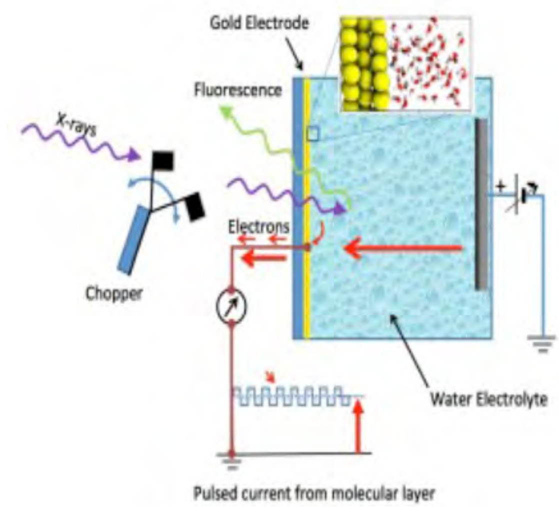

Fig. 3. ALS staff have developed tools to perform SXR XAS and XPS spectroscopies at electroechem (Science **346**, 3624 (2014).).

electronic levels that are directly involved in chemical bonding, in diverse environments and often in functioning devices. For example, the JCAP energy hub uses them heavily to understand the fundamental interfacial processes in candidate artificial photosynthetic cells (Fig. 2). Modern APXPS has been developed on beamlines ALS 9.3.1, 9.3.2, and 11.0.2 to probe, for example, catalytic reactions under realistic operating conditions and electrode surfaces in contact with an electrolyte. Commercially available APXPS capabilities are now being deployed at facilities around the world. Recent result (e.g., Fig. 3) have demonstrated the ability to do SXR at solid-liquid and operating electrochemical interfaces.

AMBER: Advanced Materials Beamline for Energy Research (AMBER) beamline, which will be enabled by repurposing beamline 6.0.2 (formerly used for femtosecond x-ray slicing), will collect many of these spectroscopies and microscopies on a single beamline for advanced preparation and multimodal analysis of energy and catalytic systems, thereby increasing ALS capabilities and providing badly needed capacity in this area. AMBER will provide *in situ* sample-preparation with SXE/resonant inelastic x-ray scattering (RIXS) and absorption spectroscopies, APXPS with high spatial resolution at near-atmospheric pressure, and a high throughput STXM capability. Construction of AMBER will be partially supported by the JCAP and JCESR Energy Hubs, the LBNL BATT program, and by partners at PNNL.

Bend magnet SXR spectroscopy beamline: To increase our capacity further in this area so as to address burgeoning user demand for these capabilities, we will update and restart ALS bend magnet beamline 7.3.1, and move a SXR spectroscopy end station from beamline 6.3.1.2.

HAXPES: The ALS has developed an intermediate energy (2-6 keV) photoemission capability on intermediate energy beamline 9.3.1. In the past year staff have used this to develop the remarkable and unique capability to measure XPS spectra at an electrode surface under a thin liquid layer. This is rapidly becoming a very popular technique, particularly for the JCAP and JCESR Energy Hubs. This old beamline is badly in need of renovation. JCESR has recently provided funds for a new vacuum crystal monochromator, and this will be installed in late 2015.

3. Multimodal Scattering Techniques: RSoXS, SAXS/WAXS, Crystallography

RSoXS: The ALS operates a unique resonant soft x-ray scattering (RSoXS – 11.0.1.2) beamline which is applied mostly to soft materials, a complementary capability to the workhorse hard x-ray SAXS-WAXS (7.3.3) beamline, and a materials crystallography beamline (11.3.1). These are heavily used to study energy materials in unusual environments, for example, microporous membranes used in batteries, fuel cells, artificial photosynthetic devices and metal organic framework (MOF) compounds proposed for gas separations, carbon sequestration, and catalytic reactors. The ALS RSoXS beamline was commissioned three years ago and has used the chemical contrast available near the carbon K-edge to probe organic and polymer thin films, notably the interfacial structure of organic transistors, heterojunction photovoltaics, and in self-assembled block copolymer films. It is has rapidly grown to become our most productive soft x-ray beamline. Supported in part by a special allocation from SUFD to ALS beamline scientist Cheng Wang, an upgrade to study liquid and complex fluid samples in several different environments is being planned and will be executed in 2016.

SAXS/WAXS: In the next 3-4 years, we plan to relocate ALS SAXS/WAXS beamline 7.3.3 to a superbend or possibly the 5.0 wiggler source with 100x higher flux at high energy. This will allow either sub-ms time resolved studies or higher energy resolution studies of bulk materials and thin films. The end station supports an increasingly diverse set of sample environments and leads our effort to handle large data streams. We have recently formed a partnership with the Molecular Foundry to streamline access for MF to this SAXS/WAXS beamline. This will mostly be accomplished through the ALS Rapid Access program started about one year ago. A new staff member has been hired jointly by the ALS and MF to help the process become successful.

High throughput materials crystallography: We have also formed a partnership with the Molecular Foundry to help fund migration of 11.3.1 to a superbend beamline over the next year to enhance our materials crystallography capabilities.. This will provide ~1000x more flux at high energy to increase capacity, precision, and to enable measuring micron-scale crystals. We will install robotic sample handling to enhance throughput and allow rapid materials screening and combinatoric experiments. This very productive beamline and the SAXS/WAXS beamline are increasingly used in ‘mail in’ and/or ‘remote access’ modes. The Molecular Foundry is now partnering on both of these and we will soon provide streamlined access by MF users.

B. Materials to Enable Ultralow Power Information Processing

Understanding the fascinating materials physics of multiferroics, oxide superconductors, graphene, topological insulators, and skyrmions, for example, is often motivated by an important practical goal: to reduce the power consumed by electronic devices ranging from transformers to microprocessors. Most future applications will involve multiscale devices that channel a signal from a nanoscale structure – few electrons on a capacitor or a nm-scale magnetic bit, for example – into the macroscopic world with high efficiency, high fidelity, and low noise. To solve this well-known electronic power consumption problem will require development of new transformative materials technologies that enable ultralow power logic elements, memory devices, power conversion devices, and beyond. The ALS supports diverse activities along the path between the fundamental electronic and magnetic properties of materials to functional electronic and magnetic devices that are very close to the market.

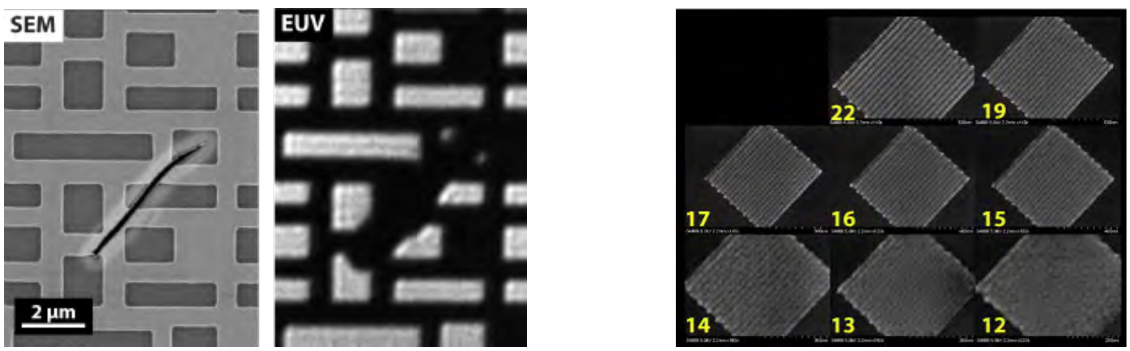

Fig. 4: Left: Imaging mask defects with secondary electron microscopy (left) and an EUV actinic inspection tool EUV. At-wavelength imaging is crucial to characterize amplitude and phase defects in multilayer masks used in EUV lithography. (Mochi, et. al., Proc. SPIE 7636, 76361A (2010). Right: Lines and spaces printed with EUV lithography down to 12 nm period. Such studies have been essential in developing EUV optics and resist materials.

1. Emerging Nanoscale Circuits: EUV lithography

The microelectronics industry has managed the power problem primarily by making smaller, lower-power transistors. Worldwide photolithography research hinges on an abrupt jump to a radically shorter wavelength range known as extreme ultraviolet (EUV), with the promise of nanoscale circuit patterns and generations of continued shrinking. Synchrotrons are among the world's brightest sources of EUV light, and the ALS, through the LBNL Center for X-Ray Optics, has emerged as a unique resource for pre-competitive EUV lithography research and technology development, fostering a number of breakthroughs over the past 15 years (Fig. 4). World-leading research programs performed in part at the ALS in optics, masks, photoresist materials, and thin-film mirror-coating technologies have defined the state of the art in this field.

SEMATECH has recently funded a major expansion of the CXRO EUV program, with installation in 2012 of a new, 100x brighter tool for at-wavelength inspection of EUV reflection masks, and in 2015 a new EUV exposure tool with a resolution limit of 8 nm coupled to a clean room with state-of-the-art semiconductor materials processing equipment.

2. Quantum and Magnetic Materials; MAESTRO, QERLIN, spinARPES, High Fields

Smaller microelectronic devices operate with lower power, but this is more than offset by the ever-increasing density of transistors on a chip: the power dissipated by a microprocessor has increased by typically 20% per year even though the energy consumed by a single logic operation has fallen exponentially with Moore's law. For this reason there is a pressing need to develop materials that enable ultralow power electronic devices. The ALS is having a major impact in this area, and Table 1 indicates even more powerful tools are planned.

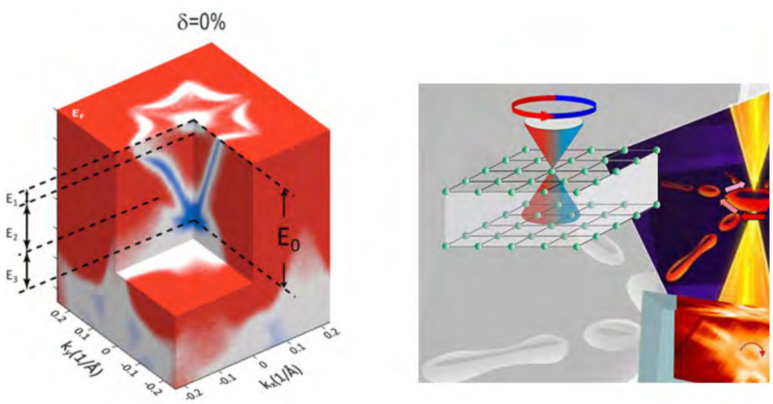

Fig. 5. First demonstration of a topological insulator by high-resolution photoemission. D. Hsieh et al., Nature 452, 970 (2008), and Y.L. Chen et al., Science 325, 178 (2009).

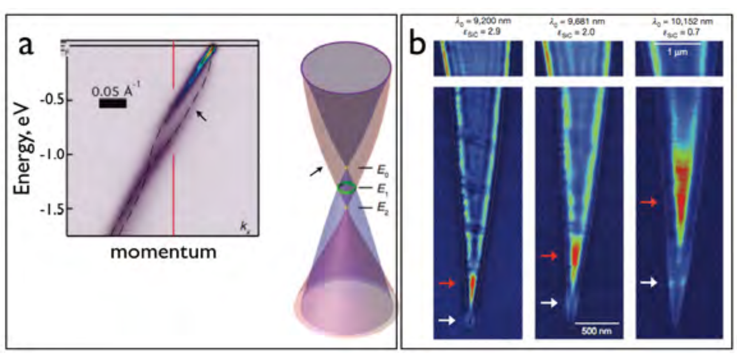

Fig. 6. (a) ARPES spectrum for a homogeneous sample of graphene shows the presence of a satellite band (indicated by the black arrow) due to plasmaronic states. Bostwick et al. *Science* **328**, 999 (2010). (b) Graphene nanostructure designed to confine plasmons (red/white arrows). Chen et al., *Nature 487, 77 (2012)*. With spatial resolution, ARPES can be used to investigate the spatial dependence of electron-plasmon coupling.

MAESTRO: The angle-resolved photoelectron spectroscopy (ARPES) program at the ALS has led the world to many important discoveries relating to pure and homogeneous materials, including work in high temperature superconductivity, giant magnetoresistance and in the discovery of properties of graphene, topological insulators (TIs) and other exciting new "Dirac" materials (Figs. 5-6). These discoveries were made possible by a continuous and ongoing program of instrumentation development in detectors, in situ sample preparation, facile data handling and analysis software, and cryogenic sample goniometry.

In the past few years, we have worked to extend this capability to probe the interplay of structure--either externally imposed through material engineering or through self-organization--with electronic properties. This has culminated in the construction of the Microscopic And Electronic STRucture Observatory (MAESTRO) beamline (Table I), which will improve the spatial resolution available at the ALS to <50 nm. Coupling such a probe to extensive thin film growth and ancillary characterization tools, users will address major problems such as the origin of self-organized structures in correlated materials; the deployment of high mobility materials such as TIs and metal-oxide heterostructures in novel device schemes; the examination of novel electronic materials such as graphene in high-field devices; the probing of multifunctional materials on the nanoscale; electronic structure of nanocrystals on an individual particle basis; the coupling of light and electronics in emergent "plasmonic" technologies (Fig. 6).

QERLIN: A strength of ARPES is that it measures the coupling electrons and holes to low energy excitations, but the results are integrated over all low energy excitations. It can be difficult to verify which excitation(s) lead to a particular exotic property. To understand what drives a particular property – high temperature superconductivity, for example – it is crucial to measure the dispersion relations of the low energy excitations directly, with high resolution, with soft x-ray contrast, and over a large region of Fourier space. For this reason, and also for the connection to nano-kinetics discussed in the next section, one of the highest ALS priorities is to develop a soft x-ray RIXS beamline called QERLIN (Q- and Energy-ResoLved INelastic scattering). We will repurpose beamline 6.0.1, the second part of the ultrafast slicing program, to develop QERLIN. QERLIN will be based on a cutting edge optical design that involves multiplexing the incident beam across the face of the sample, providing 10's of meV resolution with good signal in a very cost-effective approach.

High field magnetic spectroscopy: Resonant soft x-ray spectroscopy and scattering have also emerged as important tools in probing spin-, charge-, and orbital-ordered ground states of transition metal oxides, and the ALS has important capacity in this area as well. Table 1 includes an important augmentation of that capacity with an ARRA-funded superconducting octapole end station. This is presently being commissioned and will enable magnetic spectroscopy of oxides and hard magnet phases with fields up to 5T in arbitrary direction, thereby allowing users to probe the poorly understood anisotropy of spin- and orbital-ordered phases in complex oxides.

Magnetic and spintronic materials can be ideally studied with polarization-dependent soft x-ray techniques since these provide quantitative magnetic information with element-specificity, sensitivity to the valence state of the absorber, and the symmetry of the absorber site. Moreover, soft x-ray magnetic microscopies provide nanometer spatial resolution and time resolved measurements allow access to fundamental time scales. Over the past 15 years, scientists at the ALS have invented, constructed, and optimized unique spectroscopy, microscopy, and scattering instruments that represent new experimental capabilities and provide access to new experimental geometries that had not been explored before.

Internal spin sources and spin currents: spinARPES A key enabling issue in spintronics is to develop internal sources of spin currents. TI states, giant spin Hall structures, and half-metallic compounds are popular candidate technologies that are all actively studied by ALS users. A new spinARPES spectrometer based on ALS-developed high efficiency spin detectors is presently being commissioned on beamline 10.0.1. We will also continue to develop time-of-flight spinARPES capabilities used during two-bunch and possibly pseudo-single-bunch operation.

Magnetic STXM: An important longer term strategic priority is to develop a flexible beamline optimized for soft x-ray spectromicroscopy of magnetic materials. Some capacity in this area exists in ALS existing microscopes, but the difficulty of precision control systems with variable temperature and magnetic field and the difficulty of photoelectron emission microscopy (PEEM) with an applied field seriously limits our capacity to study magnetic materials *in situ* and magnetic devices *in operando*. Examples of systems that can be only partly studied include magnetic domain behaviors, spin ice and other patterned nanomagnetic structures, ferromagnetic and antiferromagnetic vortices, and skyrmions. The COSMIC scattering branch, in Table 1 and described in more detail in the following section, will provide a valuable probe of equilibrium or steady state magnetization dynamics. But the limit in ALS capability in imaging magnetic textures is serious. For example, most known skyrmion phases exist below room temperature and at moderate applied field and these cannot presently be well studied studied on existing ALS microscopes. The ALS is seeking funding to include in its portfolio a soft x-ray STXM dedicated to magnetic and spintronic materials (Table 1) with ~15-20 nm spatial resolution and the ability to vary temperature and applied magnetic field.

Multifunctional materials discovery: **combinatoric end station** An increasingly popular and important approach to discovering new materials is to produce combinatoric libraries, using either discrete samples or composition gradients. Such a program is particularly important in magnetic materials given their importance in many energy conversion technologies, but clearly numerous long-range goals also exist in functional oxides, lanthanide compounds, and beyond. A key feature of these efforts is to apply cutting-edge microfocused tools to probe the desired material properties quickly and efficiently, coupled to strong theory and modeling programs. For magnetic and spintronic materials, the first of these is presently being developed on ALS magnetic spectroscopy beamline 6.3.1, which is also being upgraded to provide a smaller focal spot and equipped with the necessary sample handling and, in the future, in situ growth. Also, a connection is being formed with the Materials Project at the Berkeley Lab (see https://materialsproject.org/) to provide valuable computational and theoretical guidance for this program. This effort has been planned for some time, but the rapid implementation was strongly supported by a recent crosscutting magnetism review.

C. Crossover between Atomic-Scale Dynamics and Nanoscale Kinetics

A hierarchy of length and time scales governs many important dynamical processes. For example, reconfiguration of small molecules often occurs on picosecond vibrational or femtosecond electronic times scales. In a protein molecule, however, ultrafast dynamics near a reaction center can be dramatically influenced by the longer-scale conformational changes of the protein backbone. Similarly, a spin flip at a magnetic domain wall can occur on the picosecond time scale characteristic of spin waves, but the domain wall moves much more slowly and the domain wall configuration helps control the flipping of a single localized spin.

1. SXR Chemical Dynamics and Kinetics

In chemical reactions, the dynamic-kinetic crossover occurs roughly at a time scale of $h/k_BT \sim 1$ ps. A process occurring much faster than this is dynamical, and temperature and Arrhenius kinetics are not relevant. A slower process is inherently kinetic and is often modeled statistically with, e.g., a prefactor and activation energy. By contrast, the dynamical oscillatory modes of a magnetic nanostructure can persist for times beyond 1 ns and diffusive motion characterized by kinetic rate equations dominates at longer time scale. We call the regime between these dynamical and kinetic limits the "nanokinetic" regime, which is the focus of this third ALS research theme. We seek to develop soft x-ray tools to probe nanokinetics, to establish rules that govern the interplay between dynamical and kinetic phenomena and to gain control over how a system evolves through the nanokinetic regime.

Fig. 7. The chemical reactions of Criegee intermediates important for atmospheric chemistry were studied using an apparatus at ALS Beamline 9.0.2. O. Welz et al., *Science* **335**, 224 (2012).

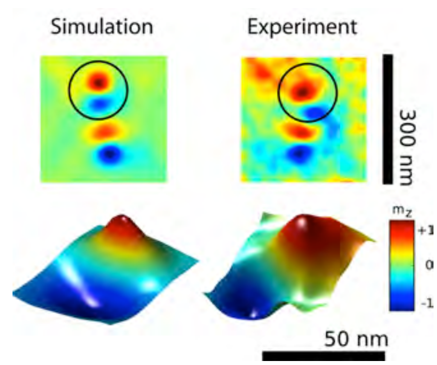

Fig. 8. Stroboscopic images of switching of coupled magnetization vortex cores in permalloy discs, measured on the ALS BL11 STXM.
A. Vansteenkiste et. al, *Nat. Phys*. **5**, 332 (2009).

The ALS has an array of tools to undertake such studies. The productive and unique ALS Chemical Dynamics program, for example, combines ALS capabilities with resources and expertise in the LBNL Chemical Sciences Division to serve an important and large user community. Examples of recent accomplishments include identification of the Criegee intermediate in combustion with spectroscopy in a flame (Fig. 7) and identifying a new path for hydrogen bonding and proton migration. In the past year the ALS has purchased a late-model SXR monochromator from the Wisconsin Synchrotron Radiation Center, and this is being installed by the LBNL Chemical Sciences Division on beamline 9.0.1 to enable ALS Chemical Dynamics program to expand the breadth and depth of their program. A multi-divisional effort led to the purchase of an untrafast high power laser support pump-probe studies of electronic and nuclear motion on the picosecond time scale. A new Approved Program is proposed to develop this new program.

2. Dynamics and kinetics in magnetic and quantum materials

A key aspect of the current ALS strategic plan is the termination of our existing programs in sector 6 based on ultrafast x-ray pulses produced with laser slicing of the electron beam. Activity in this area is rapidly migrating to free electron laser facilities, and ALS resources will be repurposed to serve communities more closely aligned with the capabilities of ring-based sources. This decision is accompanied by a plan to renew and expand our focus on nanokinetic phenomena. Several of the strategic capabilities in Table 1 reflect this change of focus and will focus directly on nanokinetic problems. A decade ago, ALS staff and users invented tools to probe magnetization dynamics with time-resolved STXM, PEEM, and full field x-ray microscopy. This strong ALS community has focused recently, for example, on magnetization dynamics in single and coupled magnetic nanostructures (Fig. 8).

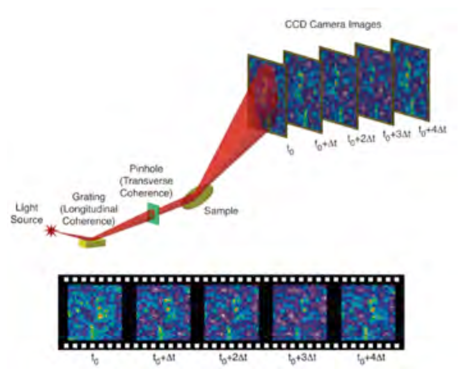

Fig. 9. Thermally driven fluctuations in the orbital-ordered phase of a complex manganite crystal using coherent soft x-ray scattering. J.J. Turner et al., *New J. Phys*. **10**, 053023 (2008).

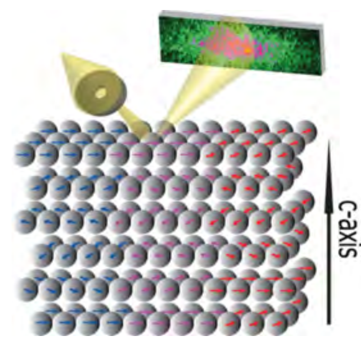

Fig. 10. Equilibrium magnetization fluctuations and domain jamming was studied in antiferromagnetic dysprosium on ALS BL 12.0.2.2 using XPCS. (S.W. Chen, et.al., *Phys. Rev. Lett*. **110**, 217201 (2013).

Nanokinetics with COSMIC: In addition to the ptychography capability discussed in Sec II.a, COSMIC will also provide a branch for soft x-ray correlation spectroscopy (XPCS, Fig. 9). This will be ideal for measuring nanoscale kinetic phenomena with resonant soft x-ray contrast to probe equilibrium, steady state, and non-equilibrium processes in chemical, magnetic systems. Experiments on the precursor beamline to COSMIC (ALS 12.0.2.2) have focused primarily on complex magnetic systems (Fig. 10), but an LDRD-funded project will enable this to expand to chemical systems to measure, e.g., catalytic kinetics in nanoporous materials like zeolytes, thereby connecting the science goals in this section to those in Sec. II.A. A crucial goal is to increase the spatiotemporal dynamic range of the technique, which depends quadratically on source brightness and coherent flux. COSMIC will expand our capabilities, but the proposed ALS-U described in Sec. III.B will provide a revolutionary expansion of XPCS.

Connecting XPCS/COSMIC with RIXS/QERLIN to probe nanokinetics: Van Hove's space-time correlation formalism of neutron and photon scattering indicates a direct relationship between correlation spectroscopy in the time domain and quasielastic scattering in the frequency domain. Indeed, the shape of the quasielastic neutron scattering peak is commonly used to probe diffusive fluctuations of overdamped material modes. In the same way, RIXS can used to probe sub-picosecond kinetics in Fourier-space. A key long-range goal of the ALS strategic plan is to connect the sensitivities of the QERLIN and COSMIC scattering beamlines to provide a revolutionary tool set to probe the nanokinetic regime.

Supporting technologies to probe nanokinetics: The first x-ray streak camera was commissioned at the ALS about 10 years ago and remains a useful capability. The change of ALS focus from ultrafast x-ray science to nanokinetics suggests numerous applications for high frame rate streak cameras with ~1 ps time resolution. For this reason we plan to re-energize our streak camera-development program to focus on both externally stimulated and thermally driven processes. This effort will need to be closely coupled to efforts focused on developing fast readout detectors – MHz and faster - since this will often determine the repetition rate that can be used. Streak cameras also offer interesting prospects to fast XPCS measurements.

D. Understanding Complex Interactions in Natural Systems

The ALS supports tools to image biological structures ranging from biopolymer molecules using macromolecular crystallography to entire organisms using x-ray tomography (Fig. 11). A similar range of environmental structures can also be probed with chemical contrast. As in the other research areas discussed here, biological and environmental systems exhibit interesting and important phenomena that involve interaction between scales. The activity of an enzymatic center is determined by the secondary and tertiary structures of a protein molecule. The complex chemistry of a soil particle is determined by the availability of various species at the interfaces.

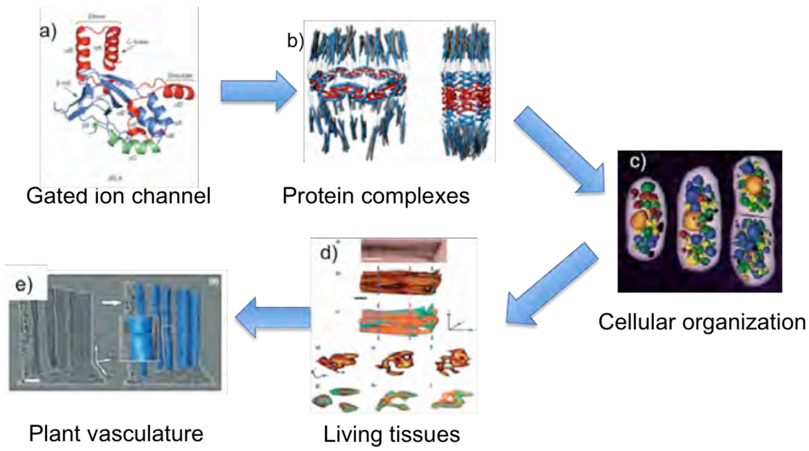

Fig. 11: The scales of structural biology illuminated by recent ALS results: a) protein structure of a gated ion channel (Brelidze, et. al., Nature 481, 530 (2012)); b) protein assembly to form the nuclear pore complex (Solmaz, et. al., PNAS 110, 5858 (2013)); c) single cell CAT scans with soft x-ray nanotomography (Parkinson, et. al., J. Struct. Biol.,162: 380 (2008)); d) infrared tomography of living tissues with few-micron resolution(Martin, et. al., Nature Methods 10, 861 (2013)); e) x-ray tomography of living grape vines(McElrone, et. al., J. Vis. Exp. 74, e50162 (2013)).

The capabilities of soft and hard x-ray techniques to address biological problems pertain mostly to the images in Fig. 11, not the arrows that connect different scales, yet these transitions between scales are of crucial importance to understanding how these complex systems function. What determines the function of a given protein molecule in a complex? How is a protein complex distributed in a cell to support and regulate cell function? How does intracellular signaling make a tissue work? We have many tools to measure biological and environmental structures over a large spatial scale, but we have mostly an empirical understanding of how these scales interact. Addressing these questions will illuminate the connection between structural and systems biology, or environmental structures and environmental systems. Emerging tools for environmental and biological science in Table 1 will help fill this crucial gap in understanding

GEMINI: The macromolecular crystallography beamlines at the ALS have enabled outstanding scientific productivity, providing high-performance hard x-ray diffraction beamlines that have kept pace with the changing needs of the structural biology community (e.g., Fig. 11(a)). To continue to provide the highest possible performance, the Howard Hughes Medical Institute has recently funded a new high brightness protein crystallography facility called GEMINI at ALS sector 2. This will significantly expand our ability to probe small crystals with large unit cells, i.e., an emphasis on protein complexes like the nuclear pore complex in Fig. 11(b). This will include a high brightness in vacuum undulator serving two branch lines simultaneously located in a single hutch. One of the branches will be served with diamond beam-splitters and operate at fixed wavelength; the other will be variable wavelength for multi-wavelength anomalous dispersion measurements. Design is underway and completion is expected in three years.

Infrared spectro-tomography of living systems: SUFD provided funds to increase ALS infrared capacity to help the NSLS community through the 'dark age' between the shut down of NSLS and the commissioning of IR beamlines on NSLS-II. Using these funds we will develop source point 2.4, reflecting the beam to the 1.4 IR end stations so that two stations can be used simultaneously. We have worked closely with NSLS staff to develop this plan and they now have an ALS Approved Program proposal to serve their users needs and to establish a presence on the ALS floor. The new IR beam will serve a full-field microscope with a focal plane array detector. Moreover, ALS staff collaborated with Carol Hirshmugl at the University of Wisconsin to develop infrared spectro-tomography at the SRC (Fig. 11(d)). This new IR station will be able to do full-field microscopy and tomography, thereby providing a new and valuable way to produce 3D images living biological and environmental systems with ~5 micron resolution and the chemical contrast of infrared spectroscopy. ALS and NSLS IR communities alike are very enthusiastic about this future; an ALS user meeting IR workshop in October, 2013 overflowed for two full days.

Biological SAXS: Protein SAXS on the ALS SIBYLS beamline, with a focus on combined SAXS/crystallography studies, is highly productive and there is a need for more capacity in this area. There is also interest in building a new soft/intermediate x-ray energy scattering beamline. The higher scattering rate at soft x-ray wavelengths will enable the highest quality time resolved measurements from small quantities of samples. Such kinetic measurements help address the structural/systems biology interface discussed above. Grazing incidence scattering provides significant information on membranes and membrane proteins. Developing these capabilities over the next several years will depend on funding raised by the bioscience community.

Nano-infrared imaging: The spatial resolution of far-field infrared imaging and spectro-microscopy is dictated by the diffraction limit. For many mesoscale scientific problems it will be necessary to resolve far smaller detail than the micron length scale probed by typical IR microscopes. Therefore, ALS staff have collaborated to pioneer the coupling of a broadband synchrotron IR beam to the tip of an atomic force microscope to enable full FTIR spectral fingerprints to be obtained with a spatial resolution only limited by the physical size of the AFM tip. Obtaining rich chemical spectra from ~20 nm scale regions is revolutionizing the depth of information obtainable for molecular interactions and materials properties on the mesoscale

Higher resolution hard x-ray tomography: The ALS hard x-ray tomography beamline provides submicron resolution tomographs that often for a useful complement to other higher resolution images (e.g., Fig. 1(a)). We are planning an upgrade of this beamline that will allow insertion of focusing optics, thereby providing ~100 nm resolution in 3D.

E. Leveraging Soft X-ray Phase Coherence

An important recommendation from the October 2014 workshop in science opportunities with high brightness SXR beams was to focus on techniques that take full advantage of phase coherence. While in some sense this is obvious, since high brightness leads to high coherent flux, the ensuing discussion has motivated attendees to think in new directions, notably interferometric detection, Fourier transform spectroscopy, and the limits of iterative phase retrieval. Some of the 2016 LBNL LDRD proposals lead by ALS staff reflect this thinking, and this is becoming a long-range ALS strategic focus. A few of the ideas being considered include

- ***High sensitivity detection***: In the optical domain, interferometric detection is often used to achieve ultrahigh sensitivity and/or precision. A good example relevant to the soft x-ray regime would be detecting and imaging pure spin currents, that is, spin currents with no net charge current, injected into non-magnetic media. Achieving this with high bandwidth would be an important step to optimizing spintronic devices, but the magnitude of the relevant circular dichroism in these situations is extremely low. Such spin currents have been notoriously difficult to detect and image. ALS staff are thinking robust SXR magnetic microscopies that operate with phase rather than (or in addition to) amplitude sensitivity. That has been done by inserting a Zernicke phase plate in the optical path of a full-field transmission x-ray microscope, but that does not actually take advantage of high brightness and full phase coherence. An obvious alternative is diffractive imaging or ptychography, where the phase is recovered from a diffraction pattern using a computer. The precision of these measurements relative to an interferometric measurement with intrinsic sensitivity to phase was discussed and needs further study. The latter is easier to signal average, which will probably lead to higher sensitivity.
- ***Fourier transform spectroscopy***: Another ambitious goal based on leveraging transverse coherence is to develop Fourier transform spectroscopy to achieve very high energy resolution resonant inelastic x-ray scattering (RIXS). High resolution RIXS is a challenging technique presently being pursued at facilities around the world, and it is an important part of the ALS Strategic Plan; it is discussed in Sec. II.B in the context of measuring coupled excitations in quantum materials, and in Sec. II.C in the context of connecting dynamical and kinetic time/energy regimes. RIXS instruments under development tend to have ~10+ meter spectrographs that will achieve modest resolution of 15-20 meV with very low signal. The QERLIN design described briefly in Sec. II.B can help improve the signal, but not the resolution. Even achieving a resolution of 1 meV will require spectrographs of unmanageable size. An alternative is develop and deploy SXR Fourier transform spectrometers, which can be very compact, can provide very high resolution, and can have larger angular acceptance than a spectrograph.

This short section at the end of this chapter on science capabilities and instruments provide a long-range focus for the ALS program and also for science on ALS-U. This illustrates where the facility and its strong user community is likely to have a major impact in the coming decades. The ALS is on the path to have that impact, especially with the proposed ALS lattice upgrade.

III. ALS-Gold: Accelerator Renewal and Upgrades to Maintain World Leadership in Soft X-ray Science and Technology

The ALS produces light over a wide spectral range for users from far infrared (IR) to hard x-rays with the core spectral region in the ultraviolet (UV) and soft x-rays region. In this core region, relevant to chemistry, catalysis, surface science, nanoscience, life sciences, and complex materials, the ALS remains competitive with the newest synchrotron radiation sources worldwide. The quality of the science program is directly connected to the performance of the accelerator complex and therefore continued upgrades of the accelerator have always been a high priority activity for the ALS.

A. Upgrades recently completed or near completion

Brightness Upgrade: A recently completed upgrade project improved the brightness of the ALS by reducing the horizontal emittance from 6.3 to 2.2 nm. This resulted in a brightness increase by a factor of 3 for bend magnet beamlines and at least a factor of 2 for insertion device beamlines. With this upgrade, the ALS has one of the smallest horizontal emittances of all operating 3rd generation light sources.

Controls/Instrumentation Upgrade: The controls and instrumentation upgrade is a four year project that is scheduled to be completed in FY15. Its goal is to replace all outdated control system hardware and software, as well as much of the beam diagnostics hardware. This will enable the ALS accelerator staff to maintain and improve the reliability of accelerator operations, reduce the effort necessary to support the control system in the future and provide improvements in performance, particularly in orbit stability. With the 20 times improved bandwidth of the new BPMs and existing corrector we expect a 2 times improvement in the fast orbit feedback system.

Storage Ring RF upgrade: The existing high power RF system was nearing the end of its useful life and spares were becoming increasingly unavailable. Therefore an upgrade project is nearing completion with the goals of long-term maintainability, higher reliability, lower electricity consumption, and sufficient power reserves for all planned additions of new undulators, better immunity to ac line transients, and better fast phase stability. The main risk factor of the system, the old Klystron, was replaced in FY12 and the project is planned to complete in FY15.

Major Storage Ring Power Supply Replacement: The original large power supplies used for the four major magnet chains in the ALS lattice had become unreliable. In addition, newer design can be more power efficient and provide better stability, thereby improving orbit stability. The last of the major power supplies was replaced in FY13.

B. Near-Term Upgrades

After the previously listed major upgrades are completed, many failure risks due to aging equipment will be retired. The largest remaining component is the injector RF system. In addition to the injector RF there will be need in the future to upgrade the 20-year-old single magnet power supplies for the 48 QF and QD magnets.

Injector RF Upgrade: The RF systems in the ALS Injector are all, with the exception of the Booster RF Amplifier, are all original to the ALS from the early 1990's. Due to their age many of these systems and in particular their components, are reaching the end of their serviceable life and in some cases, replacement parts are only available from single sources or are custom builds. Currently we have not experience significant long term outages of the system but many shorter outages and the RF group spends a significant amount of time maintaining them. It is important to reduce the risk of prolonged beam outages caused by an inability to repair and maintain these systems and components. This includes the two 24 MW based modulators and trigger thyratron, the amplifiers for the sub-harmonic bunchers, the master oscillator and distribution system, and the low level RF controllers. Upgrading these systems would not only reduce this risk but give us an opportunity to increase performance and reliability.

In addition, there are ongoing infrastructure upgrade projects, namely efforts to reduce the frequency of beam losses due to AC line voltage fluctuations, as well as efforts to improve the temperature stability of the air in the end station area, as well as to improve water temperature stability further. Several ongoing upgrades are also aiming at improving the overall energy efficiency of the ALS, both at the level of technical systems (RF, power supplies, injector operation modes), as well as building systems (HVAC).

Most of the insertion devices considered for the ALS renewal are soft x-ray elliptically polarizing (EPU) insertion devices. Other devices could be short period undulators for harder (12 keV) photons. EPUs are very popular because of the great versatility in the polarization and energy range they can provide. Along with other synchrotron facilities and exploring synergies with studies geared towards the Linac Coherent Light Source, we should explore possible avenues for improvement such as:

- Non-mechanically-moving EPUs and/or improved field shapes.
- In-vacuum EPUs.
- Cryogenically cooled permanent magnet undulators or
- Nb_3Sn based Superconducting undulators for achieving ultimate brightness in the soft x-ray range and for significantly higher brightness than now is achievable with wiggler sources for operation at 12 keV.

Pseudo-single-bunch (PSB) operation—a new operational mode at the advanced light source—can expand the capabilities of synchrotron light sources to carry out dynamics and time-of-flight experiments. In PSB operation, a single electron bunch is displaced transversely from the other electron bunches using a short-pulse, high-repetition-rate kicker magnet. Experiments that require light emitted only from a single bunch can stop the light emitted from the other bunches using a collimator. Other beam lines will only see a small reduction in flux due to the displaced bunch. As a result, PSB eliminates the need to schedule multibunch and timing experiments during different running periods. Furthermore, the time spacing of PSB pulses can be adjusted from milliseconds to microseconds with a novel "kick-and-cancel" scheme, which can significantly alleviate complications of using high-power choppers and substantially reduce the rate of sample damage. On January 28, 2014 we introduced pseudo-single bunch into user time and the first experiments are being done with the kicker set at 4 kHz.

Beyond the baseline of the almost completed brightness upgrade project, work is also investigating other possible modes of operation, including low alpha modes, which are enabled by the fact that the new sextupoles allow control of the second order momentum compaction factor. This could enable substantial improvements for THz experiments in special operation modes. To support these experiments, we also consider modifying a vacuum chamber to enable larger acceptance angles for long wavelength IR radiation. Multi parameter simultaneous optimization of the linear and nonlinear lattice with genetic algorithms is used as a tool.

Presently our vertical beamsize in the insertion device straights is just under 10 microns and our short term orbit stability about 0.6 micron (or ~6%). We are planning to reduce the coupling further and are adding a number of additional EPUs. At that point the relative orbit stability would become significantly worse. The new BPM system will allow much greater orbit stability, however to take full advantage requires a number (~20) of "fast" correctors – most likely air core magnets surrounding bellow shields and associated power supplies. Complementing the improvements to fast orbit stability with the ongoing instrumentation upgrade, we are also considering to improve the long term pointing stability of our photon beams further by supplementing the photon beam diagnostics in beamlines. Also, the new storage ring timing system can allow the distribution of more precise timing signals to those users that require it.

Enabling insertion device(s) in straight 2. There are 12 straight sections in the ALS. Currently 9 of these have insertion devices in them. The remaining 3 – sectors 1, 2, and 3 – are presently being occupied with the injection systems (straight 1), RF and multibunch feedback kickers (straight 3), and camshaft kicker and other systems (straight 2). We are currently investigating the possibility of freeing up space in straight 2 to install one or two insertion devices while retaining the essential functionality for the storage ring. Amongst the ideas being considered are more compact multibunch feedback systems, replacing the 4 injection bumps with a single multibunch kicker, and relocating equipment. In addition to freeing up space, the multibunch kicker should greatly reduce injection transients making top-off more transparent.

C. ALS-Gold: Planning a diffraction-limited upgrade of the ALS

Evolutionary increases in storage ring source brightness over the past several decades like those described above have supported a robust array of x-ray capabilities that have had a major impact on many disciplines – physics, chemistry, biology, material science, and others. A large capacity has been developed around the world and is applied to diverse cutting edge research problems. In recent years an additional, revolutionary increase in storage ring brightness has been proposed and is now being planned or pursued at facilities around the world. This increase will be accomplished by deploying storage ring lattice designs with electron beam emittance comparable to the diffraction limit of the x-rays that are produced. That is, the x-ray beams will be nearly diffraction limited, with smooth, transversely coherent wavefronts. Coherence means that all photons are 'useful' in demanding experiments that require focusing the beam into a small spot or encoding a material's heterogeneity into a far-field speckle-diffraction pattern. For this reason a diffraction limited storage ring (DLSR) is ideal for examining the nano- and meso-scale structure of materials, since they enable the highest possible spatial resolution coupled to broad temporal sensitivity and x-ray contrast mechanisms. Groundbreaking new applications to study heterogeneous materials and functional devices will be possible on a DLSR.

We have therefore started to explore various lattice concepts for an ALS lattice upgrade to a multibend achromat lattice that would provide diffraction-limited soft x-ray beams up to about 2 keV, with decreasing coherent fraction at higher energy. We are focusing in particular on the balance between transverse nonlinear dynamics, longitudinal dynamics and collective effects in an integrated way. The studies are currently at a pre-conceptual design stage and include numerical and analytical physics studies together with technology evaluation in the areas of magnets (DC+pulsed), vacuum systems, and RF systems (main and harmonic). In order to continue to serve the complementary hard x-ray community that coexists on the ALS we are also studying concepts for advanced radiation producing devices to incorporate intermediate x-ray sources into the lattice. An integral part is the optimization of possible injection schemes to enable high brightness lattices by on-axis injection. The study of possible lattice choices and accelerator technologies will be informed by parallel efforts to further develop the science case for soft x-ray diffraction limited light sources.

The goal of these design studies is to develop a firm proposal of an upgrade project in the existing ALS building and tunnel, keeping the same symmetry and location and length of all insertion device straights. The currently projected brightness envelope for this source is shown in Fig. 12.

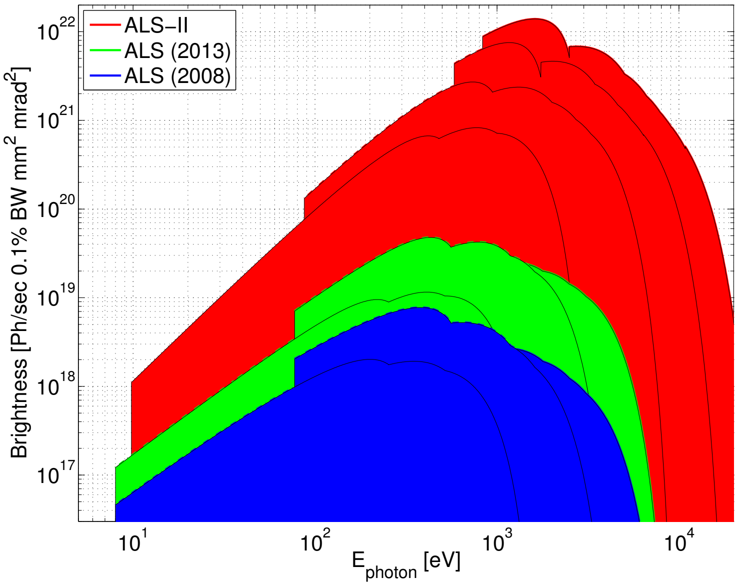

Fig. 12: Evolution of the envelope the brightness of ALS undulators. Recent upgrades have improved soft x-ray brightness by about an order of magnitude, but upgrading to a multibend achromat lattice will provide a further increase by about a factor of 100.

Such an upgrade would endow the ALS with the highest soft x-ray brightness and coherent flux of any storage-ring-based x-ray facility panned or under construction. It would manifestly increase our users ability to probe heterogeneous in ever-finer detail. It is a cost-effective upgrade that would allow a 20-year-old facility to maintain world leadership of soft x-ray science and technology for at least another 20 years.

IV. Ancillary capabilities and activities

A. Safe Operation on the ALS Experimental Floor

As part of Integrated Safety Management, the ALS Safety Program continuously evaluates the effectiveness of its program and identifies opportunities to improve. These improvements are integrated with, and support, the ALS Strategic Plan.

Integrating Floor and Accelerator Operations: ALS cross-trains floor operators, who directly work with users and who play a key role assuring safety on the floor, and accelerator operators, who would normally have limited interaction with users and floor safety. This leads to better integration of these two activities and provides more staff trained to understand safety procedures and to notice potential hazards on the floor. Similarly, there are more staff who understand safe accelerator operations. This leads to a better and more efficient operation overall. This has further evolved, with new training modules designed to further the knowledge and capabilities of all operators.

Management Walk-Arounds: ALS management schedules bi-weekly walk-arounds to understand and evaluate floor operations, with a focus on safety.

Introduction of new Work Authorization Process: The ALS has adopted a new work authorization process that combines and consolidates multiple procedures into a single system. Included in this new program is a method to evaluate electrical safety on the beamlines, incorporating the new NFPA 70E electrical safety guidelines. This will improve the evaluation of safety concerns on the floor, and facilitate improved communication to the staff about their assigned tasks and associated hazards and controls.

Beamline/Accelerator Renewals and Upgrades: The scope and nature of both beamline and accelerator projects is constantly evolving, and the EHS review processes need to evolve with them. Many projects involve upgrades of current systems and so 'abbreviated' review processes are being developed that focus resources more effectively. Also, operating experience with safety management systems such as top-off critical apertures, beamline shielding end-points, beamline radiation safety training, and other issue areas is being used to make them more effective and efficient. Lastly, current DOE trends in accelerator safety including unreviewed safety issues, configuration control, readiness reviews, etc. are being integrated into ALS processes.

Technical Capabilities: The ALS Safety Program is collaborating with other elements of the ALS in a number of areas: developing a strong user biology lab and technical support function, continuing development of chemical lab support such as glove boxes, mezzanine lab capabilities, and *in situ* capabilities for flame, low/high temperature, high pressure, laser, and other potentially hazardous environments, and improved support in the handling of low level radioactive materials.

Scientific Support: As discussed in more detail in Sec. IV.C, a primary goal of developing a new User Portal is to develop a simple and intuitive web-based input tool for users to create safety analysis forms for each of their experiments. This is being modeled on the APS system and will strive to use the same terminology and have the same outputs (controls) for similar experiments. Much of this is being piloted in the current RAPIDD project.

B. ALS Workforce Development

The success of the DOE synchrotron radiation facilities depends strongly on developing a knowledgeable and highly trained community of users and beamline scientists who apply existing tools and innovate new tools, often collaboratively, to pursue a diverse array of research frontiers. The ALS takes its role in workforce development very seriously.

The ALS takes very seriously the need to seek internal and external recognition for its scientific staff, particularly the beamline scientists who are at the heart of our success. We have regular successes on internal ALS, LBNL, and DOE awards, and we have had recent successes with external recognition as well:

- In the past year Howard Padmore was awarded the AVS Albert Nerkin Award and Fernando Sannibale was elected Fellow of the APS.
- Staff are regular recipients of annual ALS awards for excellence in research, instrumentation, and service – the Shirley, Halbach, and Renner Awards. These are awarded during the annual users meeting and selections are made by the ALS Users Executive Committee.
- With several excellent staff who have been at the ALS almost since the facility was commissioned, the ALS Division Staff Committee has placed renewed emphasis on nominating more ALS staff for promotion to LBNL Senior Staff Scientist, the rough equivalent of a full professor at a university. We achieved one such promotion last year, and are working on two such promotion cases this winter.
- ALS management focuses on developing strong candidates for DOE Early Career Awards. Our first success occurred in the past year with Alex Hexemer. A key feature of success in this was simply nominating an exceptionally strong candidate who is also an exceptionally strong, collaborative, and productive beamline scientist. We have more young candidates who fit that mold and who are nominated this year. We will continue to hone our process in the future.

External recognition for beamline staff is a more difficult problem since the portfolio of a beamline scientist does not map very well onto the criteria for external awards, which tend to be heavily oriented toward individual research contributions. The collaborative style and heavy service load of our staff (and those of other user facilities, of course) is not well matched, for example, to society awards. But our users understand and fully appreciate the efforts of our staff: the fact that the UEC regularly recognizes them with internal ALS awards provides tangible evidence for that.

As discussed above, our strongest beamline scientists establish very strong records of collaborative research, to the extent that they are equal partners with users in our strongest research activities. Postdocs with external fellowships now seek to come to the ALS to work with these strong staff in these collaborations. This is the kind of activity that allows them to establish the credentials needed to be considered for external awards. The ALS has established an awards committee composed of the Division Deputy for Science and the leaders of the

Scientific Support Group and the Experimental Systems Group, with others as needed, to focus on organizing nominations for these awards in timely fashion. We will nominate 3 or 4 of our staff for society fellowships this year. Such fellowships are an important first step, and the committee will be continuing to organize other nominations in the future.

Also important is to establish a strong pipeline of talented candidates to become facility staff in the future. Aside from the user training activities that happen daily on the experimental floor, the facility sponsors three related programs that directly impact the professional development of young scientists, from college undergraduates to advanced postdoctoral associates:

- ALS post-baccalaureate and internship program: The ALS allocates $375K/year to support undergraduate interns and recent college graduates for part- or full-time employment at the facility for a period up to one year. These students are assigned to work closely with an ALS staff scientist and to help with a project that will update or expand the capabilities of an ALS beamline or endstation. Alumni of this program are competitive in applying to the best graduate programs, and regularly select an ALS user as their doctoral thesis advisor. Other alumni have been hired for technical support positions at the ALS, elsewhere at Berkeley Lab, or in the high technology industry.
- ALS Doctoral Fellowship Program: The ALS allocates $175K/year to this program, which supports typically 8-9 doctoral fellows in steady state. This program is highly competitive and attracts superb young talent to the ALS. The ALS offers each Fellow support of about 50% of a typical graduate student pay. The Fellow's thesis supervisor generally provides the balance of financial support as well as university benefits. In addition to training, other goals of the program are to engage the thesis advisor deeply in ALS research activities and to provide a career development opportunity and supervisory responsibility to ALS staff scientists. The program was established in 2003 and has developed an impressive list of alumni.
- ALS Postdoctoral Fellowship Program: The ALS allocates $695K/year to this program, which fully or partially supports 4-6 postdocs in steady state, depending on leveraging. The strength of the ALS in applying x-rays to frontier research problems attracts a very strong pool of applicants. The financial arrangements are more diverse than for the doctoral program, but the funds are often similarly leveraged and a primary intent is again to engage faculty as well as PI's in other Berkeley Lab divisions in strong collaborations. The rapid development of ALS programs in energy science, for example, has greatly benefited from strategic allocation of these funds in collaboration with PI's in the Berkeley Lab Energy and Environmental Technology Division. About 1/3 of the alumni of this program are hired through a regular search process as a beamline scientist at the ALS or at other x-ray facilities, and a similar number are hired into faculty positions around the world and now direct their own research programs using synchrotron radiation.

There is a sizable flux of students from one of these programs into the next: a few interns and post-bacc's become Doctoral Fellows, and several Doctoral Fellows become ALS postdocs, either in the fellowship program or supported by an LDRD proposal. Given this training it is to be expected that many of the Postdoctoral Fellows continue their careers as beamline scientists or active users of synchrotron radiation facilities. These workforce development programs have a significant long-range impact on the synchrotron radiation community at large and on the ALS user program specifically, even though fellows are not allowed to engage directly in user service.

The programs have been approved and supported by the DOE and are part of the ALS FWP. The fellowship programs qualify for a significantly reduced Berkeley Lab indirect cost rate, which, combined with the leveraging described above, makes them very cost effective. The doctoral and postdoctoral programs are apparently unique among the DOE light sources. They are discussed with the ALS Scientific Advisory Committee and always receive very positive reviews.

Committees formed from the ALS staff and user community oversee these programs and help maintain a high degree of leveraging and ensure strong alignment of the programs with the facility's strategic plan. Applications for Doctoral Fellowships are solicited annually, and files are evaluated by an ad hoc committee composed of the ALS Division Deputy for Science (DDS), the head of the ALS Science Support Group, a beamline scientist and usually two faculty who conduct strong research programs at the ALS. A separate committee composed of the DDS, ALS group leaders, and two beamline scientists meets regularly to consider ALS needs for postdoctoral staffing and to evaluate applications. More detailed information about the programs, including several 'postdoc highlights', is provided on the ALS web site at

http://www-als.lbl.gov/index.php/component/content/article/56-general-resources/405-als-doctoral-fellowship-in-residence.html

http://www-als.lbl.gov/index.php/component/content/article/56-general-resources/401-als-postdoctoral-fellowship-program.html

http://www-als.lbl.gov/index.php/resources/employment/780-als-postdoctoral-fellowship-highlights.html

These workforce development programs are strongly coupled to the model the ALS uses to achieve its highly successful operation. A key ingredient of that success is career development of our beam line scientists, who through their collaborative participation in cutting edge research are highly motivated to develop new instruments and capabilities and to build a strong user program. Some of the most successful ALS beamline scientists have learned how to leverage resources available to them, including their own small beam time allocation, beam time of their close collaborators, funds from these fellowship programs, and other resources brought by their collaborators and provided by the ALS. The fellowship programs are a crucial ingredient of this process, both in supporting existing beamline scientists and training new ones.

C. Continuing Development of a Modern User Portal

The ALS User Services web interface is the first face of the ALS seen by ALS users. Provision of a modern User Services business system, for coordination of user registration, proposal administration, safety management and tracking and reporting outcomes, is essential to ensure safe and efficient user operations at ALS. ALSHub, the ALS user portal, provides a single point of entry to a personalized, easy-to-use interface which allows users and staff to:

- Register and notify ALS of arrival date
- Track status with respect to user agreements, training and ALS building access
- Submit and view current and past beam time applications,
- Submit and view current and past experiment safety documents
- Report and search for publications
- Complete all safety and security requirements and provide feedback to ALS

In order to meet ALS needs for at least the next decade, ALS has an ongoing project to further develop ALSHub to service all ALS needs related to users and to ensure the system runs on a technologically updated platform that will mitigate risks associated with older software. The ALS approach to the continuing development of the user portal is to plan upgrades, which will provide useful tools at each step. A functional analysis of the business needs has been completed and the requirements of User Services can be summarized in nine key processes (Fig. 13). Three of these processes were identified as priorities and are outlined in red and work on these is either completed (Maintain Users and Manage Experiment Safety upgrade) or is actively being worked on (Schedule Experiment).

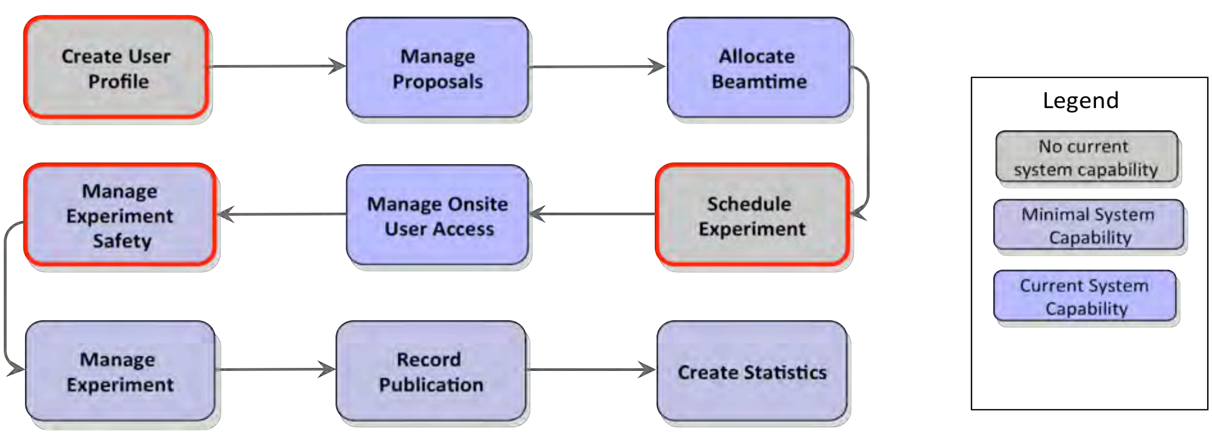

Fig. 13. Nine key processes summarize the requirements of User Services.

A centralized scheduling tool is a prerequisite for efficient flow of data from proposals through experiment safety through reporting, and should increase staff productivity. The ALS has no current centralized capability to schedule beam time; instead beam line schedules are developed independently at each beam line. This tool will provide data for ALS to manage experiment safety and will enable accurate tracking of beam line usage and optimize efficiency at each beam line. The ALS experiment scheduling system is expected to be implemented in 2016, completing the overhaul of the User Services business system.

In addition, ALS is working with LNBL to ensure that a lab-wide system under development for recording scientific publications, will be available to meet ALS needs. At this point ALS will undertake a rolling program of assessing and, if necessary, upgrading each component to ensure the user services system remains fit for purpose. Updating the user services interface for ALS users is seen as critical to ensuring safe and efficient user operations.

D. Engaging the ALS User Community to Develop a Path to Excellence

This source of this Strategic Plan is as diverse as the ALS user community because the ALS seeks regular advice from many different sources:

- We engage our Users Executive Committee (UEC) formally and informally several times per year on a host of issues to discuss how we might help users be more productive at the facility. The UEC is elected from the user population and generally represents the spectrum of research activities at the ALS.
- The UEC also organizes our annual Users Meeting, which includes typically 12-15 topical workshops organized collaboratively by our staff and users (see http://www-als.lbl.gov/index.php/user-information/users-meeting/835-2013-workshops.html). These workshops provide invaluable advice on emerging opportunities and research priorities. They are supported financially by the ALS – an indication of how valuable we think they are – and are very well attended.
- The ALS is now part of the LBNL Energy Sciences Area, the heart of DOE Basic Energy Sciences activity at the laboratory. Regular Area Meetings with partner divisions provide valuable collaborative strategic planning. For example, the ALS helped guide the discussion of potential EFRC proposals from LBNL and partnered with researchers from across the Energy Sciences area to develop these.
- The ALS has strong ties with many faculty and research groups from UC Berkeley and other UC campuses, and these also contribute to our strategic thinking.
- With oversight from our Science Advisory Committee (SAC), the ALS organizes two reviews per year of entire sub-disciplines to seek focused advice on how to optimize our capabilities to address important research problems. In the past year we have held two such reviews, one in atomic and molecular physics and another in magnetism.
- The ALS SAC, composed of national and international experts from many different disciplines, meets twice per year to provide high-level advice on our program. The ALS has enjoyed and fruitful and productive interaction with its SAC for many years. All of our strategic plans and priorities are discussed in detail with the SAC.
- The Approved Program (AP) process is another key feature of the ALS planning process. AP proposals are evaluated by the Program Study Panel (PSP), which also evaluates regular General User (GU) proposals. AP proposals must describe a research program that is of very high quality, evaluated against the GU population, and must also propose to help the ALS develop its capabilities in some significant way. The final recommendation on an AP proposal is made by the SAC, which also gauges the research and development plans in terms of the overall ALS program.
- Finally, in a fashion similar to the Approved Programs, the ALS Doctoral and Postdoctoral Programs described in Sec. IV.B provide yet another channel to engage strong users and to leverage ALS resources toward future strategic priorities.

E. Advanced Detectors

The ALS Detector Development Group builds on Berkeley Lab's history of particle detectors, in particular the past 3 decades focused on highly integrated, microelectronic-enabled detectors. The group's focus is on the development of novel soft x-ray detectors that enhance the productivity of the ALS and enhance the facility's scientific reach. Workshops (every 1-2 years) at ALS Users Meetings are forums to collect community need and interest, and, together with Experimental Systems and Scientific Support groups, drive our priorities. R&D activities are currently funded under the BES Accelerator and Detector program, and are used to initiate, design and prototype novel detector concepts. We greatly benefit from ALS Beamline 5.3.1, dedicated to detector and optics testing, as a facility to characterize and validate detector concepts. ALS operating funds are used to deploy the detectors we develop, and to adapt them to specific experiments and beamlines.

Recent activities have focused on 100s of megapixel / s direct detection CCDs developed in collaboration with the Detector Group at APS, and these have been (or are currently being) deployed at ALS, APS, LCLS, NSLS-II and XFEL. Current activities include

- Development of CCD detectors 100 times faster than those described above – currently in the prototype and evaluation phase.
- Development of very fine-pitch detectors for use in spectrographs. A 5 μm-pitch device has been produced and demonstrated, and of interest for photon-in / photon-out experiments worldwide.
- Development of very thin conductive entrance windows. Soft x-rays, at low energies, have very shallow penetration depths, so that extremely thin entrance contacts are required in order to avoid a precipitous loss in quantum efficiency. Further, to be used on fully-fabricated semiconductor detectors, the contact process must be low temperature (less than the melting point of the metal interconnects). We have developed a successful and simple process for 100 nm contacts, and are performing R&D on contacts as thin as 10 nm.
- Development of monolithic soft x-ray CMOS detectors.

Future activities are planned to include the development of sensors with avalanche multiplication (for high signal/noise soft x-ray single photon counting) and ultra-fast readout based on advances in nanometer CMOS.

As faster detectors means higher data rates, our activities are intimately connected with efforts on "big data." Both the current, straightforward, efforts at high bandwidth transport to high performance computing centers, and future R&D towards in silico algorithms for on-detector data reduction.

F. Lightsource Upgrade for X-Ray Optics Renewal (LUXOR)

The cost of new beamlines at the ALS is typically between $4M – $8M. We are now at the stage where we are starting to replace the oldest beamlines at the ALS, designed over 20 years ago. During this time, the performance of the source has radically improved in terms of brightness and stability, x-ray optics vendors can produce optics to much higher specification in more complex shapes and optical designs have become much more sophisticated.

As well as seeking funding for the complete replacements of beamlines, a prudent, rapid and very cost effective approach to lengthen the lifetime of our existing compliment of beamlines will be to invest in replacement optics typically up to 10% of the replacement cost of the beamline. These replacement optics will be of higher quality and more sophisticated design and allow us to take advantage of the current higher brightness of the ALS, compared to its brightness when these beamlines were built. We will also be able to solve many of the outstanding issues of beamline performance, where optical components have aged and are no longer operating to specification.

We have a very clear demonstration of the effectiveness of this type of optics upgrade. Five years ago, in partnership with the Berkeley Center for Structural Biology, a program was initiated to upgrade optics in three of our structural biology beamlines. The performance of these systems had decreased over the years, but by judicious replacement of key optics, we were able to gain factors of up to 100 in flux onto a small sample.

We have examined what needs to be done on all BES-funded beamlines around the ALS to bring their performance up to specification and offer a performance commensurate with the new higher brightness upgrade of the ALS. We find a range of benefits and solutions ranging from situations where no upgrade is required, on some of the newer beamlines to a situation where replacement of most optics is required, on some of the older beamlines. In the latter case, improvements of photon flux on the sample can be up to two orders of magnitude or more.

The typical cost of upgrading a beamline's optics would be around $0.5M and we could manage to do upgrades at a rate of 3 per year, so $1.5M/year. In total we would upgrade around 15 beamlines over 5 years, so a total cost of $7.5M. Early targets of this program are listed below

- Beamline 4.0: replacement of plane pre-mirror and conversion to VLS design
- Beamline 8.0: replacement of premirror, grating and refocus optics
- Beamline 10.0: replacement of gratings and pre-mirror optics
- Beamline 11.0: replacement pre-mirror, elliptical refocus mirror and branch mirrors
- Beamline 9.3.2: replacement of pre-mirror, gratings and refocus optics

We expect the upgrades above to increase resolution, throughput or stability by at least an order of magnitude over current performance.

G. State of the Art X-ray Optics Metrology Laboratory

The ALS ability to study inhomogeneous materials and material devices directly on the ability of beamline optics to transmit and focus with high fidelity the very bright ALS source onto a sample located in a complex environmental cell. Our collaboration with the CXRO to develop diffractive optics, for example, is very productive and is essential to our long-term success. A new metrology lab is also an essential ingredient of testing and aligning grazing incidence optics.

Construction of a new optical metrology laboratory in the ALS User Support Building, with comprehensive control of environmental conditions, was completed in summer 2013. Tests have shown that the lab is a cleanroom facility better than class 1,000, and with temperature stability better than +/-30 mK over a day. From late November 2013, the laboratory is in operation after the existing metrology instruments were moved from the old lab, upgraded, and recommissioned. Because the lab's capabilities now extend far beyond classical optical surface metrology to include the entire spectrum of *in situ* and *ex situ* metrology, and because it also supports the design and fabrication of x-ray optics and optical and mechanical systems, the new lab has been renamed, from the Optical Metrology Laboratory (OML) to the X-Ray Optics Laboratory.

The laboratory assures the quality of the optical components installed in beamlines or used for experimental systems. This entails measuring mirrors to ensure vendor compliance to specifications, calibrating and adjusting bending parameters for adjustable mirrors, as well as thorough alignment, tuning, and characterization of the opto-mechanical systems. Usage of different instruments *ex situ* enables us to separately investigate and address different potential sources affecting beamline performance of an optic. These are surface quality (figure and finish errors), temporal and temperature dependence of surface shape, mechanical stability, gravity effect, alignments (twist, roll-off, yaw error), etc. At the beamline, all the perturbations produce a cumulative effect to the beamline performance of the optic that makes it difficult to optimize the optic's operation performance. The *ex situ* metrology allows us to fix the majority of the problems before the installation of the optic at beamline and to provide feedback on design and guidelines on usage of optics (e.g., ambient temperature stability and accuracy of alignments).

The equipment utilized in the lab includes a phase-shift interferometry microscope, a large aperture interferometer, two slope measuring long-trace profilers, the LTP-II and DLTP, an atomic force microscope, optical microscopes, differential laser Doppler vibrometer, and various systems for development of new x-ray optics and metrology techniques. To fully realize the advantages of the new optics lab, the new high precision granite gantry system with air-bearing translation systems capable of precision 2D scanning over the surface under test (SUT) and tilting and flipping the SUT has been specified and purchased. The system (the delivery is scheduled for the end of March 2014) is a key element of the new instrument under development for surface slope metrology on the level of below 50 nrad.

H. The Data Handling and Analysis Opportunity

The need to capture, transmit, store, and analyze large volume data sets at DOE x-ray facilities and beyond has been well documented. The ALS participation in this problem is confirmed by Fig. 15, which shows the amount of raw data collected at several ALS beamlines over the past three years. In 2013, we projected that the facility will generate a total of ~2 petabytes of data. The problem is driven by a combination of high brightness sources, efficient and highly parallel detectors, and an increasing implementation combinatoric and rapid screening protocols.

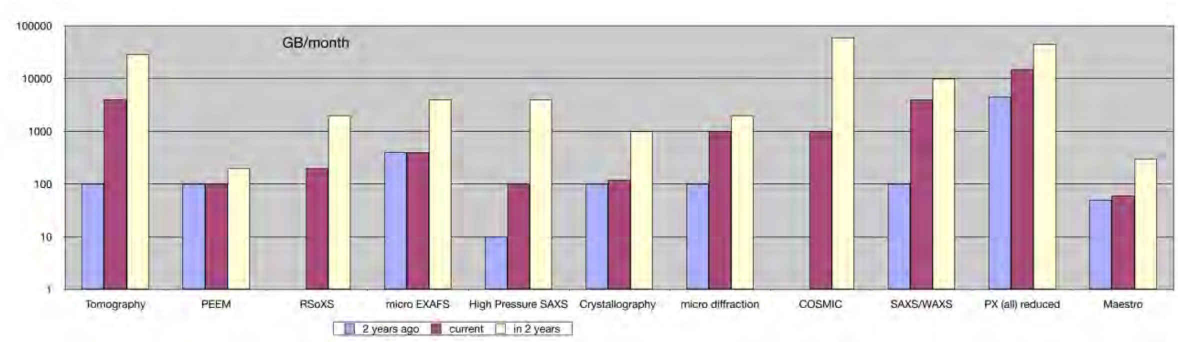

Fig. 15. Amount of raw data collected at ALS beamlines over the past three years.

Fig. 16 emphasizes the data analysis problem, which is likely the most complex part and the part that will take the most effort and time to solve. A single tomography beamline can presently produce ~10 Tb of data in a single day. Through a series of steps requiring complex software, this will be reduced to a publishable graph contained in a ~10 Mb image. The data handing capacity is being developed based on known technology, and very soon the efficiency of this process will be determined by data analysis software.

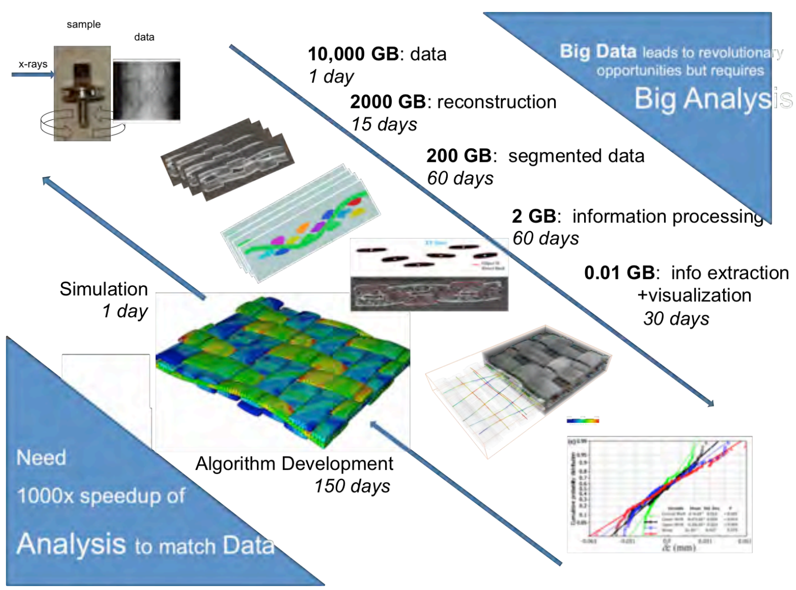

Fig 16: The path to analyzing a large data set to a publishable figure requires several steps, all of which need efficient, user friendly software that in many cases remains to be implemented.

The path to addressing the ‘big data’ problem lies in a comprehensive system of data capture, management, analysis, and integration. At a user facility, these activities are set against a backdrop of collaboration in distributed environments. With the notable exception of particle physics, state-of-the-art data capture and management infrastructures for facilities are not widely applied and high-performance data analysis pipelines are rare. Few x-ray facilities operate data archives, and none integrate data within or across facilities and its users.

In collaboration with Berkeley Lab-based and ASCR funded Energy Sciences Network (ESnet), the National Energy Research Scientific Computing center (NERSC), and the Berkeley Lab Computational Research Division (CRD) the ALS has been addressing this problem. The approach is

- to deploy advanced data transfer techniques and to make these available to the ALS community (ESnet and NERSC),
- to provide hands-free data and metadata packaging and transfer from ALS beamlines to NERSC High Performance Storage System, and
- to develop a suite of tools including 1) a robust analysis pipeline, framework, and services, and 2) on-demand data access, processing, and simulation (CRD).

Our efforts to date have focused primarily on the first two steps, in the belief that we need to establish a robust infrastructure before the third can be seriously addressed. A prototype data pipeline has been implemented on three high data rate beamlines that moves data seamlessly to NERSC and makes it available from a web browser. A fourth beamline (COSMIC imaging) is being developed with similar data management capacity. An initial suite of high performance analysis codes is being developed in four areas served by these beamlines:

- X-ray Microtomography: reconstruction code, reconstruction, image filtering and segmentation
- Grazing Incidence and Transmission Small Angle X-ray Scattering: multi-GPU code for Reverse Monte Carlo
- X-ray Microdiffraction: XMAS Microdiffraction Analysis Software
- COSMIC imaging: real-time phase retrieval for ptychographic data sets, image processing

In all of these cases, an important motivation is to increase the efficiency of ALS beamline usage by online and nearly real time (preliminary) data analysis to provide users with guidance for what to do next. We also recognize that large data sets may be useful to other researchers beyond the data generator. ALS will evolve data policies consistent with those being developed by Office of Science.

Appendix 1: List of acronyms

ALS: Advanced Light Source
ALS-U: Advanced Light Source Upgrade
AMBER: advanced materials beamline for energy research
AP: ALS Approved Program
APXPS: ambient pressure x-ray photoelectron spectroscopy
ARPES: angle resolved photoelectron spectroscopy
BATT: LBNL Batteries for Advanced Transportation Technologies program
BCSB: Berkeley Center for Structural Biology
BER: DOE Biological and Environmental Research
BER/BSISB: BER funded Berkeley Synchrotron Infrared Structural Biology Program
BES: Department of Energy Basic Energy Sciences
COSMIC: COherent Scattering and MICroscopy beamline (ALS 7.0.1 complex)
CSD: LBNL Chemical Sciences Division
CRD: LBNL Computational Research Division
DLSR: Diffraction-Limited Storage Ring
DMSE: BES Division of Materials Science and engineering
EES: LBNL Earth and Environmental Science Division
EPU: elliptically polarizing undulator
ESAF: Experiment Safety Assessment Form
ESNet: Energy Sciences Network
EUV: Extended UltraViolet lithography
GEMINI: new protein crystallography beamline
GU: ALS General User
GUP: General User Proposal
HHMI: Howard Hughes Medical Institute
HVAC: Heating, Ventilation, Air Conditioning
ISM: Integrated Safety Management
JCAP: Joint Center for Artifical Photosynthesis, a DOE Energy Hub
JCESR: Joint Center for Energy Storage Research, a DOE Energy Hub
LDRD: LBNL Laboratory Directed Research and Development
LUXOR: Lightsource Upgrade for X-Ray Optics Renewal
MAESTRO: Microscopic And Electronic STructure Observatory (ALS 7.0.2 complex)
MBA: Multibend Achromat accelerator lattice
MF: LBNL Molecular Foundry
MOF: Metal Organic Framework nanoporous material

MSD: LBNL Material Sciences Division
nanoIR: near field IR microscopy delivering ~20 nm resolution
NCEM: National Center for Electron Microscopy in the LBNL Molecular Foundry
NERSC: LBNL National Energy Research Supercomputing Center
OML: ALS Optical Metrology Laboratory
PBD: LBNL Physical Biosciences Division
PEEM: photoelectron emission microscopy
PSB: Pseudo-Single Bunch operation at the ALS
PSP: ALS Program Study Panel
QERLIN: Q- and energy resolved inelastic scattering beamline
RAPIDD: Rapid Access, Industrial, and Director Discretionary beam time proposal
RIXS: resonant inelastic x-ray scattering
RSoXS: Resonant Soft X-ray Scattering
SAC: ALS Scientific Advisory Committee
SAXS: Small Angle X-ray Scattering
SCBG: BES Chemical Sciences, Geosciences & Biosciences
SEMATECH: Semiconductor Manufacturing Technology Consortium
SINS: Synchrotron Infrared Nanoscale Spectroscopy
SISGR: DOE Single-Investigator and Small-Group Research program (2009)
SUFD: BES Scientific User facility Division
SUFD/NSLS: SUFD funding to help with NSLS dark age
spinARPES: spin-resolved ARPES
STXM: scanning soft x-ray transmission microscope
SXR: Soft X-ray
SXE: Soft X-ray Emission spectroscopy
TI: topological insulators
UEC: A:S Users Executive Committee
USUP: User Services User Portal
XAS: x-ray absorption spectroscopy
SXE: soft x-ray emission spectroscopy
SYBYLS: Berkeley Lab Structurally Integrated Biology for the Life Sciences Program
XM1: X-ray Microscope #1 (ALS beamline 6.1.2)
XPCS: x-ray correlation spectroscopy